OPTICAL QUILT PACKAGING:
A NEW CHIP-TO-CHIP OPTICAL COUPLING AND ALIGNMENT TECHNIQUE

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Abstract

by Tahsin Ahmed

Detecting trace amounts of molecules, such as early stage disease biomarkers or explosives, requires sensing with very small quantities of sample. Optical measurement is a feasible way to do the sensitive chemical or biological measurement. Specially, the mid-infrared (MIR) region (wavelength, \( \lambda = 4-12 \, \mu \text{m} \)) of the electromagnetic spectrum contains unique fingerprints corresponding to vibrational modes of molecules. Measuring the amount of light absorbed by these modes allows for highly sensitive and selective molecular detection and has generated much attention in the fields of chemical and biological sensing and explosive imaging. The recent development of the quantum cascade laser (QCL) provides a compact MIR source, feasible for incorporation into on-chip optical systems as compact and portable platforms for sensing and imaging. However, incorporating a QCL into an on-chip chemical or biological sensor, or in a beam combining platform for imaging, is challenging with the currently available techniques. While on-chip optical systems can be realized monolithically, where all
optical components (source, beam combining platform, detection medium, detector etc.) are fabricated on the QCL substrate, this scheme is not economically feasible as QCL material is very expensive (~$10k/sq-in). An alternative modular approach, where the system components are fabricated on separate substrates, requires labor extensive butt coupling, complex and expensive fiber alignment, or grating coupling to transmit light from the laser to the other system components. As a result, an improved semiconductor packaging technique for low-cost, highly efficient optical coupling is highly desirable in order to incorporate QCLs into quasi-monolithic on-chip optical systems. In this dissertation, a new and highly efficient optical coupling technique, Optical Quilt Packaging (OQP), is modeled, fabricated and characterized. OQP aligns waveguides of separate substrates by protruding, lithographically-defined interdigitated copper nodules for low-loss chip-to-chip optical coupling.

In this dissertation, the feasibility of OQP is firstly evaluated by theoretical modeling using the eigenmode expansion technique. Next, simulations are performed to quantify the coupling loss associated with the OQP devices. According to the simulation results, the optical coupling loss between a QCL laser and a low-cost Ge-on-Si waveguide can be no worse than 7 dB, when the inter-chip distance is 4 \( \mu m \) or lower. Additional waveguide geometries are also modeled to aid fabrication design and reduce the lateral misalignment loss. Next, conventional semiconductor fabrication processes are used to fabricate the first OQP chip, where two separate Ge-on-Si waveguides are aligned with an inter-chip distance of \(~4.6 \mu m\), and with a lateral misalignment of \(~1 \mu m\). Based on the simulation results, the expected coupling loss for the fabricated Ge-on-Si OQP
device is $\sim 5$ dB. The inter-chip gap is reduced further in a second OQP chip to $\sim 1.4 \mu m$, where copper alignment nodules are fabricated by sputter deposition. Finally, an MIR quantum cascade laser is used to measure the optical coupling loss of the fabricated OQP sample. The MIR light is focused to the Ge-on-Si waveguide facet and corresponding light transmission through the waveguides is measured. The OQP inter-chip coupling loss was measured to be $9.0 \pm 0.1$ dB when the inter-chip gap was in air and $4.1 \pm 0.3$ dB when filled with index-matching $\text{As}_2\text{S}_3$ glass. These results represent lower loss than previously reported chip-to-chip MIR optical coupling via butt-coupling ($\sim 10$ dB), fiber coupling (as low as $\sim 10$ dB), and grating coupling (tens of dB loss).

The initial optical coupling results suggest, OQP is a low-loss chip-to-chip MIR optical coupling technique. In the next phase of the OQP research, QCL chips will be incorporated in this new OQP fabrication process to realize an on-chip modular scheme for explosive imaging.
To my parents,

who brought me to this beautiful world,

and to my wife,

who makes my life a wonderful one...
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CHAPTER 1:

INTRODUCTION

1.1 Motivation

Photonic integration of optical sources, waveguides, and detectors is gaining popularity for applications in communications, sensing, and computing [1]–[3]. Low-cost, highly-sensitive portable devices are made possible by integrating optical sources, interaction media, and detectors. A significant challenge to photonic integration is in overcoming the difficulty integrating photonic elements that each require different substrates or incompatible fabrication processes. For example, mid-infrared (MIR) spectroscopic sensing systems are useful for detecting trace amounts of molecules, such as explosives or early-stage disease biomarkers [4], [5]. The MIR region of the electromagnetic spectrum (λ=4-12 μm) contains unique absorption “fingerprints” corresponding to vibrational modes of many molecules [6]. Measuring the amount of light absorbed by these modes allows for highly sensitive and selective molecular detection. MIR optical sensing is enabled largely by quantum cascade lasers (QCLs), which are compact, tunable, semiconductor sources that can be designed to emit throughout the MIR. Although QCLs can be incorporated into on-chip optical systems
integrating a QCL with an on-chip chemical-sensing or beam-combining platform is challenging by currently available techniques.

On-chip integrated MIR optical systems can be realized monolithically (Figure 1.1), where all optical components (source, detector, and other optical elements) are fabricated on the QCL substrate. This scheme is not economically feasible as QCL material is typically very expensive (~$10k/sq-in). Alternatively, integrated MIR optical systems can employ a modular approach where system components are fabricated on separate substrates and combined using butt coupling, fiber alignment, or grating coupling. Optical fiber coupling adds significant expense, and is especially difficult in the MIR due to a lack of commercially available fiber. Grating coupling, which is more commonly employed, suffers from high coupling loss on the order of tens of dB. Butt coupling is labor intensive and highly sensitive to mechanical vibration, leading to expensive and fragile integration [2], [3], [8]. So, the fundamental concern in creating a commercially viable optical sensor or beam combining platform is how to accomplish the integration of the various optical components in a cost effective and robust manner.

An improved semiconductor packaging technique for low-cost, highly efficient optical coupling between optical components is required to incorporate QCLs in the quasi-monolithic sensors or beam combining platforms. The ability to integrate widely disparate wavelength sources with MIR interaction or beam combining platform has the potential to open up revolutionary new applications. This dissertation will focus on the first theoretical and experimental description of a new semiconductor optical coupling scheme, called Optical Quilt Packaging (OQP), in order to address the need.
1.2 Optical Quilt Packaging (OQP)

In this dissertation, we present a new technique to apply a MEMS inter-chip semiconductor alignment and integration technique known as Quilt Packaging [9] to semiconductor optical systems. This technique, called Optical Quilt Packaging, allows for heterogeneous integration of disparate semiconductor materials into a single mechanically-stable “quasi-monolithic” chip by attaching different chips together through MEMS nodules extending from the sides of the chips. The process is compatible with industry-standard fabrication flows; is extendable to VIS, NIR, and MIR devices; can simultaneously align arrays of waveguides; eliminates manual, labor intensive alignment; and exhibits ~5 dB lower loss than manual alignment [10].

OQP achieves sub-micron waveguide alignment accuracy between two separate chips using protruding, lithographically defined interdigitated copper nodules [9], [11]. These copper nodules are placed on the sides of the chips, and can be soldered together to eliminate the possibility of misalignment due to mechanical vibration. The copper nodules are formed by filling deep-etched wells with sputter-deposited copper, then...
etching lanes to partially expose the nodules (Figure 1.2). Copper is used since it is mechanically stable, commonly available in semiconductor integrated circuit fabrication, and can thus be used to also carry inter-chip electrical signal and power [9]. Separate waveguide chips are then combined by connecting each set of copper nodules together, like a “zipper” or “LEGOs.” Using OQP, arrays of waveguides on separate chips can be aligned simultaneously. Optical waveguide chips, which are made with a combination of common MIR group IV or III-V materials, can be combined into a single heterogeneous platform via OQP following standard fabrication processes [10]. Modern lithography can have alignment accuracies of 10-100 nm, which will support IR-Vis-UV wavelengths with OQP. THz technology will require less alignment accuracy, so OQP is also compatible with THz coplanar waveguides. OQP has the unique capability to align arrays of waveguides between two separate chips. No current interchip technique can achieve uniform coupling between waveguides. The copper nodules are designed in a way such that aligning them accurately simultaneously align the waveguide arrays of the corresponding chips. Currently available waveguide array coupling techniques are expensive compared to OQP, not compatible in MIR, and requires to fabricate the interconnect between the waveguides individually [12]. Additionally, waveguide array butt coupling techniques are not capable of mechanically aligning waveguide arrays with uniform reduced coupling loss.
OQP allows direct optical interconnects (i.e., without external waveguides) between semiconductor optical sources, on-chip beam-combining optics, optical waveguides, and detectors (Figure 1.3). This technique could be used to realize on-chip compact optical sensing platforms for sensitive, low-cost monitoring of chemical and biological species. Also, beam combining from an expensive QCL array to a less expensive semiconductor waveguide array can be done by OQP for imaging of trace amounts of explosives. OQP leverages advances in Quilt Packaging (QP) [9], an electronic packaging interconnect technique wherein contacts are formed along the vertical faces of integrated circuit die, and are then joined to form electrically conductive and mechanically stable chip-to-chip contacts (Figure 1.4). The world record low inter-die insertion loss of less than 0.1 dB from 50 MHz to 100 GHz [13] with submicron alignment has been demonstrated with Quilt Packaging.
Figure 1.3: Modular MIR sensor with OQP.

Figure 1.4: SEM micrograph of an interlocking quilt packaging nodule structure [9].
OQP inherently provides the following:

1. Extremely wide spectral coverage with sources ranging from the visible, infrared, and mid-infrared
2. Separately optimized optical sources, interaction mediums, and detectors
3. Significant cost reduction compared to the monolithic integration of a source, interaction medium, and detector
4. Robustness with no free space optics, fiber coupling/epoxy, or moving parts for wavelength tuning
5. Compatibility with multiple photonic integrated sensing and microfluidic technologies.

OQP will be an enabling technology for a new class of portable, high-performance, and low-cost on-chip sensing systems. In this dissertation, detailed simulation and fabrication work on OQP will be shown along with optical measurement of coupling. The future applications with OQP will also be discussed at the end of the dissertation.

1.3 Waveguide Platform for Beam Combining

In MIR trace explosive detection, light from laser sources will be coupled into inexpensive, low-loss waveguides on separate chips for beam combining. While MIR waveguides can be fabricated either on InP or the substrate containing the QCL heterostructure, silicon substrates are a preferred platform for OQP waveguide technology due to the low cost of materials and fabrication via established fabrication processes. Several promising material technologies are compatible with MIR OQP, as summarized in Table 1.1. MIR on-chip waveguides will be formed by defining a ridge or rib [14] of a
higher index of refraction material (core) on top of a lower index of refraction material (cladding), so that light is confined to propagate along the length of the core (confined by the lower cladding layer and the outermost air layer). Ge-on-Si waveguides (Figure 1.5) can extend the operating range of silicon MIR photonics with losses as low as 2.5 dB/cm at $\lambda \approx 14 \mu m$ [15]. Also, Ge-on-Si waveguides have recently been demonstrated as an on-chip optical sensor for drug testing for law enforcement agencies. Ge-on-Si waveguides are fabricated with traditional semiconductor fabrication steps, which are compatible with OQP [2]. For these reasons, Ge-on-Si is selected as the beam combining platform in this OQP research.

**TABLE 1.1**
LOW LOSS TRANSMISSION WINDOW FOR SEVERAL MIR OPTICAL MATERIALS [14]–[16]

<table>
<thead>
<tr>
<th>Material</th>
<th>Wavelength Range loss &lt; 1 dB cm$^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Si_3N_4$</td>
<td>0.22 $\mu m$ – 6.6 $\mu m$</td>
</tr>
<tr>
<td>Si</td>
<td>1.2 $\mu m$ – 6.9 $\mu m$</td>
</tr>
<tr>
<td>$Al_2O_3$ (sapphire)</td>
<td>0.25 $\mu m$ – 4.3 $\mu m$</td>
</tr>
<tr>
<td>Ge</td>
<td>1.9 $\mu m$ – 16.7 $\mu m$</td>
</tr>
<tr>
<td>$SiO_2$</td>
<td>2.9 $\mu m$ -3.6 $\mu m$</td>
</tr>
<tr>
<td>$As_2S_3$ (chalcogenide glass)</td>
<td>0.6 $\mu m$ – 8 $\mu m$</td>
</tr>
</tbody>
</table>
1.4 Dissertation Outline

In this dissertation, a systematic approach used in realizing OQP is described. This includes a theoretical discussion of guided mode optics as it relates to OQP, numerical feasibility studies, the fabrication process, and the results from experimental characterization.

In Chapter 2, the eigenmode expansion technique is used to determine the fundamental requirements to be fulfilled by OQP for successful optical coupling. The electromagnetic propagation physics is discussed first [17]–[19], and then the Helmholtz equation for TM (transverse magnetic) wave propagation is used to find the guided optical modes. Also, mode matching between the guided modes of separate waveguides
is used to predict the effects of inter-chip gap and waveguide misalignment on optical coupling.

Chapter 3 describes the feasibility simulation of OQP using an open source software package called MEEP (MIT electromagnetic equation package) [20]. The simulation results determine the inter-chip gap and waveguide-to-waveguide misalignment tolerance for successful chip-to-chip optical coupling.

Chapter 4 presents the detailed fabrication process to build the OQP coupled waveguide chips. As the first test device, a Ge-on-Si to Ge-on-Si OQP device is fabricated. The detailed fabrication process is described. The relevant fabrication challenges with the solutions are described for the Ge-on-Si OQP device. To develop the current fabrication process and make it compatible with QCL chips, an improved copper nodule fabrication technique is proposed and realized.

In Chapter 5, the optical measurement technique regarding OQP coupling is described. Measurement challenges are discussed with the solutions. Also, the coupling loss measurement results with a Ge-on-Si passive OQP device are discussed in detail.

Chapter 6 discusses the future research opportunities with OQP. At the end of the chapter, OQP research progress until now is summarized.
CHAPTER 2:
EIGENMODE ANALYSIS OF OPTICAL WAVEGUIDE

2.1 Introduction

In this chapter, an eigenmode expansion technique is used to develop a mathematical model of chip-to-chip optical coupling via Optical Quilt Packaging. This mathematical model is then used to gain insight into the expected performance and limitations of OQP. As mentioned in Chapter 1, OQP is a scheme for highly-efficient waveguide coupling that is suitable for direct optical interconnect between semiconductor optical sources, optical waveguides, and detectors via waveguides. OQP leverages the advances in Quilt Packaging (QP) [9], an electronic packaging technique wherein contacts formed along the vertical faces are joined to form electrically-conductive and mechanically-stable chip-to-chip contacts. In OQP, waveguides of separate substrates are aligned with sub-micron accuracy by protruding lithographically-defined copper nodules on the side face of a chip. The goal in OQP is to align waveguides of separate chips with minimum misalignment and with minimum inter-chip distance to reduce coupling loss. Eigenmode expansion is used as a fast numerical technique to define the goals of OQP [17], [18]. In this chapter, the Helmholtz equation
of TM (transverse magnetic) mode is used to find the eigenvalues and eigenvectors associated with the propagation. Modal overlaps between guided modes of separate waveguides are used to predict the effects of inter-chip gap and waveguide misalignment on optical coupling. In the eigenmode expansion technique, a 2-dimensional slab waveguide structure is analyzed and the numerical analysis is done with Matlab. This approach is taken to develop a fundamental understanding of wave propagation in a waveguide, the type of modes associated with the propagation, and the effect of mode matching in optical coupling.

2.2 Eigenmode Expansion Technique for a Three Layer Slab Optical Waveguide

In a QCL, the wave propagates in the TM mode [19], [21]. Therefore, our eigenmode expansion analysis will only consider TM mode propagation in this chapter. The goal of the analysis is to calculate the modal overlap between the laser and Ge-on-Si waveguide modes to predict optical coupling. Additionally, beam divergence characteristics in the inter-chip air-gap will be analyzed to determine the associated optical loss. The analysis will set up the initial criteria for efficient optical coupling.

To understand the eigenmode expansion, a simple three layer slab optical waveguide with a two-dimensional structure is considered initially (Figure 2.1). The refractive indexes of the three layers are considered as \( n_1, n_2 \) and \( n_3 \). The structure is considered uniform in the \( y \) and the \( z \) direction. For a Ge-on-Si waveguide structure, the three layers become: (1) cladding (air): \( n_1 = 1 \); (2) core (germanium): \( n_2 = 4 \); and
Figure 2.1: A three-layer slab Ge-on-Si waveguide.

(3) substrate (silicon): \(n_3 = 3.42\). The refractive indexes of Ge and Si mentioned here are for 8 \(\mu m\) wavelength of MIR light, which is relevant to many MIR chemical and biological applications [22]. According to the boundary conditions of Maxwell's equation, the tangential \(E\) and \(H\) field components are continuous for two adjacent media (valid for \(H\) field if there is no current flow in the medium) [19]. As a result, Helmholtz equations can be used for the analysis, which are considered for uniform media (see Appendix A.2, equation (A.33) and (A.35)). The three-layer structure is uniform in the \(y\) direction, so it can be assumed that, \(\frac{\partial}{\partial y} = 0\). So, the Helmholtz equations for the \(E\) and \(H\) field can be expressed as [8] (Appendix A.2 for the detail discussion):

\[
\frac{d^2 E}{dx^2} + k_0^2(\varepsilon_r - n_{\text{eff}}^2)E = 0,
\]

(2.1)
Before discussing the TM mode propagation in the $z$ direction, first the component representation of the Maxwell's equation is described for better understanding of the analysis. From the phasor representation of Maxwell's equations (see Appendix A.2, equation (A.12) and (A.13)), the components of the electromagnetic fields are related to each other by [8]:

$$\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} = -j\omega\mu_0 H_x,$$  
(2.3)

$$\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = -j\omega\mu_0 H_y,$$  
(2.4)

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = -j\omega\mu_0 H_z,$$  
(2.5)

$$\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} = j\omega\epsilon_0\epsilon_r E_x,$$  
(2.6)

$$\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} = j\omega\epsilon_0\epsilon_r E_y,$$  
(2.7)

$$\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} = j\omega\epsilon_0\epsilon_r E_z.$$  
(2.8)

Now, for the TM mode, the longitudinal $z$ direction component of the magnetic field is 0 ($H_z = 0$), but the transverse $y$ direction component of the magnetic field is not 0 ($H_y \neq 0$). The structure is uniform in $y$ direction, so $\frac{\partial E_y}{\partial x}$ becomes 0. As a result, $E_y$ is constant and can be assumed as 0. Then, using $H_z = 0$ and $E_y = 0$ in equation (2.7), $\frac{\partial H_x}{\partial z}$ also becomes 0. So, $H_x = 0$ can be assumed. Thus, in TM propagation [23]:

$$H_x = H_z = E_y = 0.$$  
(2.9)
So, the following equation for the principle magnetic field component describes the TM mode propagation:

\[
\frac{\partial^2}{\partial x^2} H_y(x) + k_0^2 (\varepsilon_r(x) - n_{eff}^2) H_y(x) = 0. \tag{2.10}
\]

Next, the eigenmode expansion technique is used to find the optical modes in the three-layer slab system. The eigenmode expansion technique is a powerful numerical technique for waveguide modeling compared to finite-difference time-domain (FDTD), finite element method (FEM), and beam propagation method [24]. Eigenmode expansion calculates optical modes associated with an optical waveguide structure faster than the other mentioned methods. In Eigenmode expansion, the electromagnetic propagation is simulated by decomposing the electromagnetic field into its basis eigenmodes. In linear algebra, a non-zero vector \( \mathbf{x} \), is an eigenvector of a square matrix \( \mathbf{A} \), if the following relation holds:

\[
\mathbf{A} \mathbf{x} = \lambda \mathbf{x}, \tag{2.11}
\]

where \( \lambda \) is a scalar eigenvalue associated with the eigenvector \( \mathbf{x} \). For \( n \times n \) operator matrix \( \mathbf{A} \), there would be \( n \) eigenvalues of the linear system with \( n \) number of corresponding eigenvectors. In order to find out the eigenvalues and the corresponding eigenvectors associated with the electromagnetic field, the equation (2.10) is modified to have the form of equation (2.11). The following steps are done to modify equation (2.10):

\[
\frac{1}{k_0^2} \frac{\partial^2}{\partial x^2} H_y(x) + (\varepsilon_r(x) - n_{eff}^2) H_y(x) = 0
\]
\[
\Rightarrow \frac{1}{k_0^2} \frac{\partial^2}{\partial x^2} H_y(x) + \varepsilon_r(x) H_y(x) = n_{\text{eff}}^2 H_y(x)
\]

\[
\Rightarrow \left[ \frac{1}{k_0^2} \frac{\partial^2}{\partial x^2} + \varepsilon_r(x) \right] H_y(x) = [n_{\text{eff}}^2] H_y(x) \quad (2.12)
\]

\[
\Rightarrow \frac{1}{k_0^2} H_y''(x) + \varepsilon_r(x) H_y(x) = [n_{\text{eff}}^2] H_y(x) \quad (2.13)
\]

\[
\Rightarrow AH_y(x) = \lambda H_y(x). \quad (2.14)
\]

Now, equation (2.10) can have a linear form like equation (2.11), if the second-order derivative part of equation (2.13) becomes linear. The finite difference method is used to get the approximate linear form of the second order derivative. If the \( H_y \) field has discrete values \( \Delta x \) apart from each other along the \( x \) axis, the centered three point model for second derivative becomes:

\[
H_y''(x_j) = \frac{H_y(x_{j-1}) - 2H_y(x_j) + H_y(x_{j+1})}{\Delta x^2}, \quad (2.15)
\]

where

\[
\Delta x = x_{j+1} - x_j = x_j - x_{j-1}.
\]

Now, if the \( x \) axis is discretized into \( n \) points such that, \( x = x_1, x_2, x_3, \ldots, x_n \), then from equation (2.13) and (2.15), the following equation sets can be written:

\[
\begin{align*}
\frac{1}{k_0^2} \frac{H_y(x_0) - 2H_y(x_1) + H_y(x_2)}{\Delta x^2} + \varepsilon_r(x_1) H_y(x_1) &= [n_{\text{eff}}^2] H_y(x_1), \\
\frac{1}{k_0^2} \frac{H_y(x_1) - 2H_y(x_2) + H_y(x_3)}{\Delta x^2} + \varepsilon_r(x_2) H_y(x_2) &= [n_{\text{eff}}^2] H_y(x_2), \\
\vdots \\
\frac{1}{k_0^2} \frac{H_y(x_{n-1}) - 2H_y(x_n) + H_y(x_{n+1})}{\Delta x^2} + \varepsilon_r(x_n) H_y(x_n) &= [n_{\text{eff}}^2] H_y(x_n),
\end{align*} \quad (2.16)
\]
or

\[
\begin{align*}
\frac{1}{k_0^2 \Delta x^2} H_y(x_0) &+ \frac{2}{k_0^2 \Delta x^2} \varepsilon_r(x_1) H_y(x_1) + \frac{1}{k_0^2 \Delta x^2} H_y(x_2) = [n_{eff}^2] H_y(x_1), \\
\frac{1}{k_0^2 \Delta x^2} H_y(x_1) &- \frac{2}{k_0^2 \Delta x^2} \varepsilon_r(x_2) H_y(x_2) + \frac{1}{k_0^2 \Delta x^2} H_y(x_3) = [n_{eff}^2] H_y(x_2), \\
\ldots \\
\frac{1}{k_0^2 \Delta x^2} H_y(x_{n-1}) &+ \frac{2}{k_0^2 \Delta x^2} \varepsilon_r(x_n) H_y(x_n) + \frac{1}{k_0^2 \Delta x^2} H_y(x_{n+1}) = [n_{eff}^2] H_y(x_n).
\end{align*}
\]  
(2.17)

Equation set (2.46) has the following eigenvalue equation form:

\[
AH_y(x) = \lambda H_y(x)
\]

where

\[
\lambda = n_{eff}^2,
\]

\[
A = \begin{bmatrix} 
\frac{2}{k_0^2 \Delta x^2} - \varepsilon_r(x_1) & 1 \\
\frac{2}{k_0^2 \Delta x^2} & -\frac{2}{k_0^2 \Delta x^2} - \varepsilon_r(x_2) \\
\frac{1}{k_0^2 \Delta x^2} & \frac{2}{k_0^2 \Delta x^2} - \varepsilon_r(x_n) \\
\frac{2}{k_0^2 \Delta x^2} & - \frac{1}{k_0^2 \Delta x^2} \\
\end{bmatrix}
\]

and

\[
H_y(x) = \begin{bmatrix} 
H_y(x_1) \\
H_y(x_2) \\
\ldots \\
H_y(x_{n-1}) \\
H_y(x_n)
\end{bmatrix}
\]
Now, in the operator matrix $A$, the three input parameters are: (1) vacuum wavenumber $k_0 = \frac{2\pi}{\lambda_0}$, (2) relative permittivity $\varepsilon_r(x) = n^2(x)$, and (3) the step size of discretization $\Delta x$. The operator matrix $A$ is constructed with the input parameters to solve the eigenvalue problem and find out the eigenvalues $\lambda = n_{eff}^2$, and corresponding eigenvectors. In the eigenvalue solution, the eigenvectors represent the $H_y(x)$ field profile of the optical modes. The wavelength for the simulation is chosen as $\lambda_0 = 8\mu m$, a wavelength in the mid-infrared transmission window which corresponds to many MIR biological, medical and environmental applications [15][6]. For the initial simulation, a distance of $20 \mu m$ along the $x$ direction is chosen with a step size of $\Delta x=0.1 \mu m$. Since this matrix approach assumes $E$-field is zero outside of the simulation region, the boundary conditions are two metal walls. This is valid for modes where the $E$-field goes to zero at the boundaries, as in guided waveguide modes. Explicitly, the boundary conditions for the simulation are $H_y(x < 0.1 \mu m) = 0$ and $H_y(x > 20 \mu m) = 0$. The relative permittivity $\varepsilon_r(x) = n^2(x)$ is defined along the $x$ direction. The relative permittivity for the Ge-on-Si waveguide layers are (Figure 2.2):

$$
\varepsilon_r(x) = n^2(x) = \begin{cases} 
11.70; & 0 < x \leq 8 \mu m \text{ (Si substrate),} \\
16; & 8 < x \leq 12 \mu m \text{ (Ge core),} \\
1; & 12 < x \leq 20 \mu m \text{ (Air cladding).}
\end{cases}
$$

So, a Ge-on-Si slab waveguide with a $4 \mu m$ thick Ge core is considered in this case.
Next, the operator matrix $A$ is constructed in Matlab using $\text{diag}$ function. With the recent computational speed increase in computers, Matlab can solve eigenvalue problems for large $n \times n$ operator matrix very quickly. For an example, a $1000 \times 1000$ operator matrix can be solved in $\sim 1$ second. In the initial simulation, there are 200 points along the $x$ axis ($x = 0.1 \mu m$ to $20 \mu m$, with step size $\Delta x = 0.1 \mu m$), so the $200 \times 200$ operator matrix ($\mathbf{A}$) is constructed. As $200 \times 200$ operator matrix $A$ is used in the simulation, the Matlab $\text{eig}$ function returns the first 200 eigenvalues and their corresponding eigenmodes. The effective index ($n_{\text{eff}}$) values are obtained by square rooting the eigenvalues.

![Figure 2.2: Modes in Ge-on-Si waveguide.](image)
TABLE 2.1
EFFECTIVE INDEX VALUES FOR GE-ON-SI WAVEGUIDE

<table>
<thead>
<tr>
<th>First 20 effective index (n_{eff}) values for Ge-on-Si waveguide</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. 3.918</td>
</tr>
<tr>
<td>6. 3.051</td>
</tr>
<tr>
<td>11. 0.967</td>
</tr>
<tr>
<td>16. 0+ i 1.699</td>
</tr>
</tbody>
</table>

For the Ge-on-Si waveguide simulation, the first 20 effective index values are given in Table 2.1. The n_{eff} value determines the type of mode associated with it. The detailed mathematical explanation of how n_{eff} values are used to determine the mode type is discussed in Appendix A.3 [25]. The most relevant waveguide mode for power propagation is the guided mode. In the guided modes, the field profile \( R(x) \) is oscillatory in the waveguide core region, which decays exponentially in both substrate and cladding region [25]. The power is conserved in guided modes as the electromagnetic wave propagates along the z direction in the waveguide (Figure 2.1). The 'red' and 'green' field profiles shown in Figure 2.2 represent two guided modes of the Ge-on-Si slab waveguide. The dashed 'blue' line is the first substrate mode. The substrate mode profile (shown in Figure 2.2) does not represent the actual profile, since the boundary condition considered here is not ideal (i.e., in an actual Ge-on-Si waveguide the substrate is much thicker than 8 \( \mu m \)). Also, substrate modes do not carry
any guided power, so they are neglected in the optical coupling calculation. The relationships between the mode type and the effective index values are summarized in Table 2.2.

The eigenmode expansion can be used to find out the mode profiles in an optical waveguide. In this chapter, the goal of the eigenmode expansion is to find out the criteria for successful optical coupling between the source waveguide (QCL) and the passive waveguide (Ge-on-Si). So, the eigenmode analysis is done with the InP QCL structure in Section 2.3. Next, the effect of the inter-chip gap on optical coupling will be discussed in Section 2.4.

**TABLE 2.2**

THE RELATION BETWEEN MODE TYPE AND EFFECTIVE INDEX \( (n_{eff}) \) VALUE

<table>
<thead>
<tr>
<th>Relation between mode type and effective index ( (n_{eff}) ) value</th>
<th>Mode type</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n_{core} &gt; n_{eff} &gt; n_{subrate} &gt; n_{air} )</td>
<td>Guided</td>
</tr>
<tr>
<td>( n_{core} &gt; n_{subrate} &gt; n_{eff} &gt; n_{air} )</td>
<td>Substrate</td>
</tr>
<tr>
<td>( n_{core} &gt; n_{subrate} &gt; n_{air} &gt; n_{eff} )</td>
<td>Radiation</td>
</tr>
</tbody>
</table>

2.3 Optical modes in an InP Quantum Cascade Laser

In this section, eigenmode expansion is used to determine the optical modes in an InP QCL. The relative permittivity profile of the InP QCL that is used in the simulation is shown in Figure 2.3 (with the laser structure) [26]. The laser structure consists of an
InP substrate layer, an active core region of periodic $\text{In}_{0.52}\text{Al}_{0.48}\text{As}$ barrier and $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ well layers, coupled of $n$-doped $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ layers sandwiching the active core, an InP upper cladding layer, and an InP cap layer. Once the relative permittivity (or the refractive index) parameters are known for the layers of the QCL, the optical modes can be found easily by eigenmode expansion. The first three modes of the InP QCL are shown in Figure 2.4. There are two guided modes in the InP QCL structure, and the third mode is a substrate mode. In a QCL, the laser gain occurs in the active core region. In the center of the active region, the fundamental mode ($M_0$) has peak value and the second guided mode ($M_1$) has a zero value. As a result, only the fundamental mode of the QCL is amplified, and the emission from the laser can be considered as single mode. Hence, in the mode matching analysis, it is sufficient to consider only the fundamental mode of the QCL as the source mode to determine optical coupling.

Figure 2.3: Relative permittivity ($\varepsilon_r$) profile in QCL with the cross section of the laser structure.
2.4 Propagation in the Air Gap

In this section, the mode matching method is used to determine the misalignment effect on optical coupling. In OQP, the aligned waveguides either touch at their facets, or there is an air gap in between them. In this section, the inter-chip air gap effect on optical mode matching will be discussed. Here, InP QCL is used as the source, and Ge-on-Si is used as the passive waveguide. The mode matching method calculates the match between the fundamental mode of the laser and the guided modes of the Ge-on-Si waveguide. The air gap effect on the matching can be analyzed by determining the beam propagation characteristics in the air. As light propagates in modes, the mode profile in the air can be described as ([23]):
\[ H_{y_{-air}}(x, z) = \sum_m c_m H_{y_{-air}, m}(x) \exp(-j\beta_m z), \] (2.18)

where \( c_m, H_{y_{-air}, m}(x) \) and \( \beta_m \) are the amplitude, the field profile, and the propagation constant of mode \( m \), respectively. The \( c_m \) values depend on the mode match between the \( m \) mode in the air and the QCL source mode. If the source mode (QCL mode) is denoted by \( H_{y_{-QCL}}(x) \), the amplitude of the excited mode \( m \) in air \( H_{y_{-air}, m}(x) \) is calculated as [23]:

\[ c_m = \int_{-\infty}^{\infty} H_{y_{-QCL}}(x) \ H_{y_{-air}, m}(x) dx, \] (2.19)

or numerically as:

\[ c_m = \sum_{i=0}^{n} H_{y_{-QCL}}(x_i) \ H_{y_{-air}, m}(x_i). \] (2.20)

Figure 2.5: Illustration of the inter-chip air gap in between the InP QCL and Ge-on-Si waveguide.
Now, if $z$ is considered 0 at the QCL-air gap interface, the $H_{y-QCL}(x)$ at $z = 0$ can be expressed as the weighted superposition of all the air modes:

$$H_{y-QCL}(x, 0) = \sum_{m} c_m H_{y-air,m}(x) = H_{y-air}(x, 0). \quad (2.21)$$

The QCL fundamental mode has a Gaussian like field profile as shown in Figure 2.4. So, the beam propagation in the air gap should follow Gaussian beam characteristics. As discussed in Section 2.2, two metal layers are considered at the $x$ direction boundaries in the eigenmode analysis. As metal reflects electromagnetic waves, the simulation length along the $x$ axis is increased to 200 $\mu$m in order to avoid any interference effect from the reflected beam. For the modal analysis of wave propagation in the air gap, first the optical modes in the air are calculated. The first 3 modes in the air are shown in Figure 2.6. Next, following equation (2.20), the mode amplitude coefficients ($c_m$) are calculated. The first 400 mode amplitude coefficients are plotted in Figure 2.7. Once the mode amplitude coefficients are calculated, the $H_{y-air}(x, 0)$ field profile can be matched with the laser $H_{y-QCL}(x, 0)$ field profile at their interface $z = 0$ by using equation (2.21). There are 2000 points along the $x$ axis in the air eigenvalue calculation ($x = 0.1 \mu m$ to $x = 200 \mu m$ with a step size of 0.1 $\mu m$), so the solution has 2000 eigenvalues and 2000 mode amplitude coefficients ($c_m$). The $c_m$ values get close to 0 at the $c_{400}$ point (Figure 2.7). So, in order to achieve the profile matching, it is sufficient to use only the first 400 $c_m$ values. The matched $H_y(x)$ profiles are shown in Figure 2.8. It is evident from the plot that the $H_{y-air}(x, 0)$ (dashed blue line) field profile perfectly overlaps with the $H_{y-QCL}(x, 0)$ field profile (solid red line).
Figure 2.6: Optical modes in the air gap (first 3 modes).

Figure 2.7: Amplitude coefficients of the excited modes (first 400 coefficients).
After matching the field profiles at the laser-air interface, the TM propagation profile in the air can be calculated with equation (2.18). The time variation can also be calculated by the following equation:

\[
H_{\text{air}}(x, z, t) = \sum_m c_m H_{\text{air},m}(x) \exp(-j \beta_m z) \exp(j \omega t)
\] (2.22)

The electromagnetic propagation considered in the analysis is a time harmonic one, so the \( \exp(j \omega t) \) term repeats periodically. As a result, equation (2.18) alone can be used to calculate the TM field profile in the air gap. The \( H_{\text{air}}(x, z) \) profile is plotted in Figure 2.9. The profile displays a diverging characteristic similar to a Gaussian beam in free space [27], which is shown in Figure 2.10. Now, for a diverging Gaussian beam, the
Figure 2.9: Beam propagation in the air gap.

Figure 2.10: Beam radius of a diverging Gaussian beam [28].
beam radius \( w(z) \) at a distance \( z \) from its minimum value \( w_0 \) is [25]:

\[
w(z) = w_0 \sqrt{1 + \left(\frac{z}{z_R}\right)^2},
\]

(2.23)

where

\[
z_R = \frac{\pi w_0^2}{\lambda_0}.
\]

(2.24)

Here, beam radius is considered as the distance from center of the beam, where the peak intensity is decreased by the factor \( 1/e^2 \approx 0.135 \) [27]. The beam radius at \( z = 0 \) is considered as \( w_0 \). In our simulation, \( w_0 \) corresponds to the beam waist of the \( H_{-air}(x,0) \) (or \( H_{-qcl}(x,0) \)) field intensity. From the \( H_{-air}(x,0) \) field intensity profile (Figure 2.11), the minimum beam radius is found as \( w_0 = 1.95 \mu m \). The field intensity is calculated from the multiplication of the field and its complex conjugate. From the corresponding field intensity profiles (Figure 2.12), the beam radius at \( z = 10 \mu m \) is \( W(z = 10) = 12.25 \mu m \), and at \( z = 20 \mu m \) is \( W(z = 20) = 28.55 \mu m \).

For comparison, \( w(z) \) values are also calculated using equation (2.23) (Figure 2.13). The calculated beam radius values from the plot are \( 13.2 \mu m \) and \( 26.19 \mu m \), at \( z = 10 \mu m \) and \( z = 20 \mu m \), respectively. So, the TM propagation through the air gap, which is shown in Figure 2.9, loses its Gaussian characteristics with the propagation. This occurs due to the interference effect, which is introduced by the reflected wave from the metal boundaries. So, the decay of the Gaussian characteristic can be reduced by increasing the simulation length along the \( x \) direction (i.e., increasing the metal boundary distance).
Figure 2.11: Beam intensity at the QCL-air gap interface.

Figure 2.12: Beam intensity profile, (a) at $z = 10 \mu m$, and (b) at $z = 20 \mu m$. 
2.5 QCL to Ge-on-Si waveguide optical coupling

In this section, the optical coupling from the QCL to Ge-on-Si waveguide will be calculated using mode matching. The fundamental mode of the QCL and the TM propagating mode profile in the air gap have already been calculated. Now, the mode matching technique is used to find out the power delivered from the QCL fundamental mode to the Ge-on-Si guided modes through the air gap. The air gap propagation is calculated using equation (2.18). As shown in equation (2.21), the QCL fundamental mode and the superposition of the air modes match at $z = 0$. So, this superposition of the air modes can be considered as the QCL mode propagating along the air gap (i.e., $H_{-qcl}(x) = H_{-air}(x)$ along $z$ direction). Then, the power transferred from the QCL...
fundamental mode to the two Ge-on-Si guided modes can be calculated as (* denotes complex conjugate):

$$
Power_{Ge-on-Si,\text{guided}} = (c_1 H_{-Ge,1}(x) + c_2 H_{-Ge,2}(x)) \times (c_1 H_{-Ge,1}(x) + c_1 H_{-Ge,2}(x))^* \\
= c_1^2 |H_{-Ge,1}(x)|^2 + 2c_1c_2 H_{-Ge,1}(x) H_{-Ge,2}(x) + c_2^2 |H_{-Ge,2}(x)|^2 \\
= c_1^2 + c_2^2
$$

(2.25)

; [H (x) is an eigenvector, so, $H_{,m}(x) \times H_{,n}(x) = 0$ when $m \neq n$, and $|H_{,m}(x)|^2 = 1$].

Now, calculating the values of $c_1^2$ and $c_2^2$ (the values vary with $z$), the power transferred to each of the guided modes and the total transferred power is found (Figure 2.14). Interestingly there is no power transferred to the second guided mode of the Ge-on-Si waveguide. Both the QCL and the Ge-on-Si fundamental mode are even functions with respect to the center of the waveguide core, but the second guided mode of Ge-on-Si is an odd function. As a result, the power is only transferred to the fundamental mode (first guided mode) of the Ge-on-Si waveguide. The transmitted power is a measurement of optical coupling between the InP QCL and Ge-on-Si waveguide. Optical coupling variation with inter-chip gap is plotted in Figure 2.14. According to the plot, coupling loss increases with the increase of inter-chip distance (more than 50% power is lost at an inter-chip gap of 5 $\mu m$). As a result, the OQP technique should be able to reduce the inter-chip gap in order to reduce optical coupling loss (the best optical coupling is possible with 0 inter-chip gap).
Next, the eigenmode analysis is used to find the effect of misalignment between the core regions of the waveguides. So far, perfect alignment is considered between the centers of the core regions. Now, a gradual misalignment is introduced between the core regions from 0 to 4 $\mu m$ (with step of 0.1 $\mu m$). The power transferred to the first and second guided modes of the Ge-on-Si waveguide from the QCL fundamental mode is calculated with a 0 inter-chip gap. The result of the misalignment simulation is shown in Figure 2.15. The coupling efficiency reduces with the increase in misalignment (more than 50% power is lost at a misalignment of 2 $\mu m$). So, another requirement to be fulfilled by OQP is to reduce misalignment between the waveguides. Here, vertical misalignment is introduced between the waveguides. The lateral misalignment effect on optical coupling is similar, which will be discussed in Chapter 3.

Figure 2.14: Optical coupling between QCL and Ge-on-Si waveguide.
Figure 2.15: Optical coupling variation with misalignment between waveguide cores.

The eigenmode expansion simulation concludes with the following observations:

1. Optical coupling depends on the inter-chip gap between two aligned waveguide chips. Optical coupling decreases with the increase of inter-chip gap. As a result, for high efficiency coupling, the inter-chip gap should be reduced as much as possible.

2. Misalignment between the waveguides reduces optical coupling. So, misalignment should be reduced as much as possible in order to reduce optical coupling loss.

Eigenmode expansion simulation sets the fundamental requirements for OQP techniques. In Chapter 3, FDTD simulation is done to quantify the fundamental requirements for OQP. FDTD technique will be used in a 3-dimensional numerical
simulation in order to quantify the expected optical coupling loss associated with the OQP technique.
3.1 Introduction

In this chapter, finite-difference time-domain (FDTD) simulations are used to explore the feasibility of the chip-to-chip waveguide coupling via Optical Quilt Packaging (OQP). OQP is a proposed scheme for highly-efficient waveguide coupling and leverages advances in Quilt Packaging (QP) [9]. In OQP, waveguide arrays of separate substrates are aligned with sub-micron accuracy by protruding lithographically-defined copper nodules on the side face of a chip. As discussed in Chapter 2, in OQP, high efficiency chip-to-chip optical coupling depends on the alignment of waveguides of separate chips at sub-micron level alignment accuracy and on reducing chip-to-chip distance. In this chapter, the feasibility of OQP is investigated by calculating the optical coupling loss between butt-coupled waveguides using a free software called MIT electromagnetic equation propagation (MEEP) [20]. Simulations in this chapter are performed to determine coupling loss as a function of lateral, vertical, and axial alignment between QCL and Ge-on-Si waveguide structures. The measured coupling losses compare favorably with other conventional off-chip optical coupling techniques.
3.2 FDTD Modeling using MEEP

In FDTD simulation, space and time are divided into grids, and the time evolution of Maxwell’s equations is performed. FDTD solves the time-derivative Maxwell’s equations in an anisotropic medium, which can be written in the following form:

\[ \frac{\partial B}{\partial t} = -\nabla \times E, \quad (3.1) \]
\[ \frac{\partial D}{\partial t} = +\nabla \times H - J, \quad (3.2) \]

Here \( E, H, D, B \) and \( J \) are the electric field, the magnetic field, the electric flux density, the magnetic flux density, and the electric-charge current density, respectively. In a rectangular co-ordinate system, these equations can be expressed as [29]:

\[ \frac{\partial E_i}{\partial t} = \frac{1}{\varepsilon} \left( \frac{\partial H_k}{\partial j} - \frac{\partial H_j}{\partial k} - \sigma E_i \right) \quad (3.3) \]
\[ \frac{\partial H_i}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_j}{\partial k} - \frac{\partial E_k}{\partial j} \right) \quad (3.4) \]

Where \( i, j, k \) are the three components of the spatial co-ordinate system, \( \varepsilon \) is the permittivity of the material, \( \mu \) is the permeability of the material, and \( \sigma \) is the charge density. MEEP staggers the electric and magnetic fields in time and space, using the standard Yee discretization. Each field component is sampled at different spatial locations offset by half a pixel. This allows the time and space derivatives to be...
formulated as center-difference approximations [29]. In MEEP, boundary conditions are implemented by adding ideal absorbing boundaries around the computation cell. Absorbing boundaries are handled by perfectly matched layers (PML), which is the fictitious absorbing material that in theory absorbs electromagnetic waves at all frequencies and angles of incidence without reflecting any of them. PML added around the edges of the cell is used to shorten the computational regions in the numerical simulation with open boundaries [30]. In order to parallelize the calculation, and to efficiently store auxiliary fields only in certain regions (like PML), MEEP further divides the grid into regions, which are joined together into an arbitrary topology via boundary conditions. The computational cell is further subdivided into convex rectilinear regions. Different regions may be stored at different processors in a parallel computer [20]. In MEEP, the inputs are dielectric function $\varepsilon$ (defines the waveguide geometry), and an initial electric field component $E_i$ at a specific location of the waveguide to start the simulation. The outputs are the electric-field components ($E$) at different time slices in all locations of the computation region formulated by the standard Yee discretization. The output in MEEP is in h5 file format, which can be analyzed and visualized with a wide variety of programs, that support the hdf5 format. The h5 files can be converted by these programs to png images or 3D volumetric data files for visualization.
3.3 Simulation Results

As discussed in Chapter 2, OQP needs to overcome the challenges of precise lateral, vertical, and axial alignment for successful heterogeneous coupling between QCL and semiconductor rib waveguides with different mode geometries. Therefore, simulations will be performed to determine coupling loss as a function of lateral and axial alignment between QCL and waveguide structures. Vertical alignment was not simulated as such errors can be eliminated using conventional optical flip-chip packaging techniques [31] or wafer planarization/thinning processes with submicron-precision. In the simulation, transmission between a typical QCL ridge waveguide and a multi mode Ge-on-Si rib waveguide (8 $\mu$m wide and 4$\mu$m high) is performed for MIR light ($\lambda = 8 \mu m$ [21][15]). The chosen wavelength is in the mid-infrared transmission window, which corresponds to strong interaction with the fundamental vibrational and rotational modes of the chemical bonds in molecules relevant to biological, medical and environmental applications [32]. The MIR applications we are interested with does not require single mode optical coupling, as a result multimode waveguide dimensions is chosen [2], [3]. The simulation results with regards to coupling loss as a function of alignment inaccuracy are discussed in the following sections. Firstly, coupling loss due to inter-chip gap is examined. Then the effect of the lateral misalignment between an InP QCL and a Ge-on-Si waveguide on optical coupling loss is explored. The feasibility of using a horn-shaped waveguide geometry in the receiving end of the coupled waveguides to decrease coupling loss is also explored in the later simulations.
3.3.1 Coupling Loss Variation with Inter-chip Distance

In this section, numerical simulation is done to determine the effect of inter-chip gap on coupling loss. The eigenmode expansion study shows coupling loss increases with the increase of inter-chip gap. Now, MEEP is used to numerically quantify the loss. In the simulation, chip-to-chip separation is varied from 0 (contact) to 10 $\mu m$, in order to calculate the coupling loss as a function of inter-chip distance (Figure 3.1). The $E$ field is initiated at plane $A$ of the InP QCL side, and the output flux is measured at plane $B$ (Figure 3.1). Coupling loss is calculated by the following equation:

$$L_P = 10 \log_{10} \left( \frac{P}{P_0} \right) dB,$$

where $P$ = flux measured at the output of Ge-on-Si waveguide (at plane $B$) and $P_0$ = flux measured at the output of a QCL waveguide with a length equal to combined QCL and Ge-on-Si waveguides.

The simulation result of coupling loss variation with inter-chip gap is shown in Figure 3.2. The result indicates that the coupling loss is no worse than 7 dB for a gap of less than 4 $\mu m$ (half wavelength in this case), and is comparable to the conventional off-chip coupling [2]. Also, OQP coupling loss is reduced to 2 dB when the inter-chip gap is 0.5 $\mu m$, which is feasible with OQP technology if waveguides can be touched at their facets. The initial OQP device will combine Ge-on-Si waveguide to Ge-on-Si waveguide (will be discussed in Chapter 4), so the coupling loss variation with inter-chip gap for Ge-on-Si OQP structure ($50 \mu m$ wide and $4 \mu m$ high in both side) is also simulated using MEEP. The Ge-on-Si waveguide width is chosen $50 \mu m$ to increase the lateral modal
Figure 3.1: Inter-chip distance between an InP QCL to a Ge-on-Si waveguide.

Figure 3.2: Coupling loss variation with inter-chip gap (for $\lambda = 8 \, \mu m$).
overlap between the aligned waveguides. The coupling loss characteristic with the Ge-on-Si OQP structure is shown in Figure 3.3 [10]. According to the simulation results, coupling loss is dominated by the two following effects:

1. The transmission has a peak at half-wavelength inter-chip distance as the reflecting facets of InP QCL and Ge-on Si waveguides form a Fabry–Pérot cavity in the inter-chip gap.

2. Coupling loss increases with inter-chip distance as a result of beam divergence.

As a next step, the feasibility of filling the inter-chip gap with an index-matching material in order to decrease coupling loss is explored by FDTD simulation.
3.3.2 Index-matching Material in the Inter-chip Gap

As the simulation results show in Section 3.3.1, coupling loss increases with increasing inter-chip distance for 8 \( \mu m \) wavelength light. One of the main sources of loss is facet reflections (i.e., impedance mismatch) between the semiconductor and air at the facets, and another one is beam divergence as light leaves the laser facet aperture. Therefore, filling the gap between waveguides with an index-matching material to reduce facet reflections and beam divergence is proposed (Figure 3.4). In the simulations, an inter-chip gap of 10 \( \mu m \) (between a QCL and a Ge-on-Si waveguide) is filled with index matching materials of refractive indices, \( n = 1 \) to 4, with a step size of 1. Simulation results (Figure 3.5) show that the coupling loss decreases for higher refractive index material. So, OQP with index-matching material enables highly efficient optical coupling. The coupling loss varies from 3.44 dB to 2.10 dB for index matching material of refractive indices between 2 to 3. A similar simulation result is also shown.

![Figure 3.4: Index-matching material inserted within the inter-chip gap.](image-url)
Figure 3.5: Coupling for transmission from an InP QCL waveguide to Ge-on-Si ridge waveguide with inter-chip gap filled with different index matching material.

Figure 3.6: Coupling for transmission from a Ge-on-Si to a Ge-on-Si ridge waveguide with inter-chip gap filled with different index matching material.
for the Ge-on-Si OQP (50μm wide and 4μm high) device in Figure 3.6 [10]. Arsenic trisulfide (As₂S₃) chalcogenide glass has an index of refraction of ~2.4 in the MIR [33]. Also, As₂S₃ chalcogenide glass can be incorporated in OQP as a spin-on glass when dissolved in an appropriate solvent. As a result, As₂S₃ is a suitable candidate to be used as an index-matching material in OQP. Additionally, As₂S₃ could be utilized to fabricate mid-infrared chalcogenide glass waveguides for chemical sensing applications [34].

3.3.3 Horn-shaped Waveguide for Coupling Loss Reduction

Horn-shaped waveguide provides high efficiency coupling in integrated optics for optical transitions between planar or wide-channel waveguides [35]. In this section, horn-shaped Ge-on-Si waveguide is examined for improved coupling and alignment tolerance. The horn width and length (Figure 3.7) are varied to find the optimized transmission condition. In the simulation, the horn length is varied from \( L = 8 \mu m \) to \( L = 16 \mu m \), with a step size of 2 \( \mu m \), for a chip-to-chip separation of 4 \( \mu m \) (half of the wavelength used in the simulation). For each of the horn length, simulation is performed for horn width \( W = 8 \mu m \) to 16 \( \mu m \), with a step size of 2 \( \mu m \). Simulation results are presented in Figure 3.8. The result suggests coupling loss is minimum when the horn width is 12 \( \mu m \) (1.5 times the waveguide width without the horn).

Next, the effect of horn-length on coupling loss is explored. In the simulation, horn width is fixed at 12 \( \mu m \), and horn length is varied from \( L = 8 \mu m \) to \( L = 20 \mu m \) with a 2 \( \mu m \) step size. The chip-to-chip distance is kept at 4 \( \mu m \). The coupling loss is reduced with increasing horn length up to \( L = 16 \mu m \) (2 times the waveguide width...
without horn), but not much after that, which is shown in Figure 3.9. Coupling loss is reduced from 4.10 dB to 3.68 dB with the optimized horn length \( L = 16 \mu m \) and horn width \( W = 12 \mu m \), which is a 0.4 dB reduction in coupling loss. With the optimized horn geometry, coupling loss sensitivity to lateral misalignment between the InP QCL and Ge-on-Si waveguides is investigated next. For the optimized 12 \( \mu m \) wide and 16 \( \mu m \) long Ge-on-Si horn-shaped waveguide (for 8 \( \mu m \) wavelength light), the lateral misalignment between the waveguides is varied from 0 to 2 \( \mu m \) with a step size of 0.5 \( \mu m \). The results are compared to those of a rectangular-shaped waveguide. The changes in coupling loss for both rectangular and horn waveguides are plotted in Figure 3.10. It is evident that the coupling loss of a horn-shaped waveguide is less sensitive to lateral misalignment than that of a normal rectangular-shaped waveguide.

Figure 3.7: Horn-shaped Ge-on-Si waveguide geometry.
Figure 3.8: Coupling loss with varying horn length and width (chip-to-chip separation = 4 μm).

Figure 3.9: Coupling loss with horn length (chip-to-chip separation = 4 μm).
Figure 3.10: Coupling loss variation with horn-shaped and rectangular waveguide for lateral misalignment.

3.4 Simulation Visualization of MIR Wave Propagation

The $E$-field output is stored in MEEP as an h5 file. In order to visualize the light coupling between the QCL InP waveguide to Ge-on-Si waveguide, the h5 files are converted to vtk files. Then the vtk files are converted to png images using Paraview [36] (a free 3D visualization software tool from Sandia National Lab) to visualize the $E$-fields. In Figure 3.11, an effective coupling between the QCL to Ge-on-Si waveguides is shown using this technique. The red and blue colors represent the positive and negative $E$-field component of the 8 $\mu m$ light, respectively. This step-by-step visualization confirms that the measured light flux in the simulations is actually transmitting through the Ge-on-Si waveguide, but not through the Si substrate. This result is particularly
In Figure 3.11, infrared light of 8 μm wavelength is being coupled from InP QCL waveguide to Ge-on-Si waveguide. This is important as the Ge-on-Si waveguide substrate Si is also transparent in the MIR region of the electromagnetic spectrum.

### 3.5 Conclusion

Transmission between a typical OQP coupled QCL ridge waveguide and a single-mode Ge-on-Si waveguide is calculated to have a loss of 2 dB with an inter-chip gap of 0.5 μm and to be no worse than 7 dB for a gap of less than 4 μm. The results compare favorably with conventional off-chip coupling. In order to further increase the coupling...
efficiency and reduce sensitivity to alignment, a horn-shaped Ge-on-Si waveguide is proposed. When the horn is 1.5 times wider than the width of the waveguide, and 2 times longer than the width of the waveguide, the coupling loss is further reduced by 0.42 dB. Also, when the horizontal misalignment increases, coupling loss of the horn-shaped waveguide increases at a slower rate than that it does in a ridge waveguide. The OQP technique can be translated to other wavelengths and applications. To estimate performance at other wavelengths, simulation results presented in this chapter can simply scaled by the wavelength. For an example, if a laser of 1 μm wavelength is used, the coupling loss should not be less than 7 dB for an inter-chip gap lower than 0.5 μm if same waveguide materials are used (the refractive index varied with wavelength as well, which will require some more adjustments to be made in this approximation). The results of the simulations are summarized in Table 3.1 and in Table 3.2.

Initial simulation results suggest good feasibility of OQP as an efficient technique for direct chip-to-chip optical coupling. If submicron precision alignment can be implemented with a reduced inter-chip distance, OQP could offer good prospect in wide-bandwidth, highly-efficient waveguide coupling. With improved design of copper nodules, the inter-chip gap could even be reduced to ~1.5 μm, realizing OQP a perfect candidate for an improved chip-to-chip optical butt coupling.
### TABLE 3.1

**SIMULATED OPTICAL COUPLING LOSS FOR OQP TECHNIQUE**

<table>
<thead>
<tr>
<th>OQP Coupling Tolerance</th>
<th>1 dB loss</th>
<th>3 dB loss</th>
<th>5 dB loss</th>
<th>10 dB loss</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inter-chip distance (μm)</td>
<td>0</td>
<td>0.75</td>
<td>3.75</td>
<td>9.5</td>
</tr>
</tbody>
</table>

### TABLE 3.2

**COMPARISON OF COUPLING LOSS FOR A BUTT-COUPLED INP QCL TO GE-ON-SI WAVEGUIDE WITH AND WITHOUT HORN FOR 4 μM INTER-CHIP GAP**

<table>
<thead>
<tr>
<th>OQP Coupling Tolerance for lateral misalignment (μm)</th>
<th>Without horn (dB)</th>
<th>With horn (dB)</th>
<th>Reduction in Loss (dB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>4.09</td>
<td>3.68</td>
<td>0.41</td>
</tr>
<tr>
<td>0.5</td>
<td>4.12</td>
<td>3.69</td>
<td>0.43</td>
</tr>
<tr>
<td>1</td>
<td>4.21</td>
<td>3.73</td>
<td>0.48</td>
</tr>
<tr>
<td>2</td>
<td>5.71</td>
<td>3.88</td>
<td>1.83</td>
</tr>
</tbody>
</table>
4.1 Introduction

In this chapter, the detailed fabrication process of the Optical Quilt Packaging (OQP) technique is presented. Two Ge-on-Si waveguide chips are fabricated and aligned to demonstrate the feasibility of OQP fabrication. Ge-on-Si to Ge-on-Si OQP chip is fabricated as the initial test device, since QCL material is very expensive to perform the initial tests. The fabricated waveguides are aligned via protruded copper nodules, which are located on the side face of the waveguide chips. Finite-difference time-domain (FDTD) simulations, which are discussed in Chapter 3, suggest highly-efficient waveguide coupling is possible by reducing inter-chip distance, and by reducing the horizontal and vertical misalignment of the aligned waveguides to a sub-micron level. The Ge-on-Si OQP device is fabricated to attain these goals. The detailed fabrication process is described in the following sections, along with the relevant technical challenges and the solutions.
4.2 OQP Process Flow

The OQP fabrication process follows the general outline below, and is described in Figure 4.1:

1. Alignment nodules are defined by deep reactive ion etching (DRIE).
2. Alignment nodules are filled with copper (Cu), and chemical mechanical polishing (CMP) is used to polish the excess copper layer.
3. Waveguides are fabricated in the polished sample.
4. DRIE etch is used to make two waveguide chips from the initial sample; the copper nodules are released at the same step.
5. Alignment of the waveguide chips is done to finalize the OQP device.

Figure 4.1: Process flow for OQP. (a) Define trenches, (b) electroplate and chemical mechanical polish (CMP) copper, (c) lithographically define and etch optical components, (d) expose nodules via DRIE and separate the chips, (e) separated die, (f) mechanically combine chips.
These fabrication steps are inspired from the previous fabrication work in University of Notre Dame on "Quilt Packaging®" [9], [13], but several modifications are made to fulfill the requirement of sub-micron waveguide alignment for high-efficiency optical coupling.

In order to make the initial Ge-on-Si to Ge-on-Si OQP test device, the following three photolithography steps are performed. The combined mask layout of these steps is shown in Figure 4.2:

1. Litho 1: Fabricating copper nodules - blue patterns in the layout.
2. Litho 2: Fabricating double-trench Ge-on-Si waveguides - red patterns in the layout.
3. Litho 3: Separating the waveguide chips - pink area of the layout.

Figure 4.2: Ge-on-Si OQP device mask layout.
The fabrication steps of OQP are discussed in the following section along with the relevant technical challenges and the solutions.

4.2.1 DRIE for Defining the Copper Nodule Trenches

In the first fabrication step of the OQP sample, high-aspect-ratio trenches are formed in Ge-on-Si chips to define the copper nodule structure and size. An Alcatel 601E inductively coupled plasma reactive ion etch (ICP-RIE) system is used to perform a Bosch process [37], [38]. The Bosch process is a high speed and high aspect ratio Si/Ge etching technique that uses fluorine chemistry. Two different gases are used in the etching process: (1) SF$_6$ for the etching cycle, and (2) C$_4$F$_8$ for the passivation cycle. The etching and the passivation cycles are used independently one at a time, which is shown in Figure 4.3.

During the etching cycle, a shallow isotropic profile is formed due to SF$_6$ discharge on the Si substrate. Next, during the passivation step, a protective fluorocarbon film is formed on the primarily etched surface due to C$_4$F$_8$ discharge. During the next etching cycle, ion bombardment preferentially removes the fluorocarbon film from the horizontal surface, but leaves the protective film in the sidewall. As a result of these alternating cycles, a highly anisotropic feature is built, which is shown in Figure 4.4. The Bosch process in the DRIE has an alternating etching cycle and a passivation cycle of about 7 seconds and 2 seconds, respectively. The Bosch
Figure 4.3: Typical Bosch process with etch and passivation cycle. For Si and Ge etch SF$_6$ flow rate of 300 sccm of 7 seconds and C$_4$F$_8$ flow rate of 130 sccm for 2 seconds are used, respectively [38].

The Bosch process works best at about 20° C. At this temperature, the selectivity is very high between Si and standard photoresist masks reaching around 200:1. The selectivity is even higher (exceeding 300:1) for a large variety of hard masks (SiO$_2$, Si$_3$N$_4$, etc.) [39]. In the DRIE system, the Bosch process has an SF$_6$ flow rate of 300 sccm and a C$_4$F$_8$ flow rate of 130 sccm. The pressure is set at 23% by the position of automatic pressure control. The source power is 1800 W, and the substrate power is 80 W, during the plasma generation. The system uses nitrogen cooling to maintain the temperature of the Si substrate/sample at around 20° C.
In the copper nodule trench fabrication lithography step, photoresist AZ 1813 is used. The resist is spun twice at a speed of 4000 rpm for 35 seconds to form a ~2 μm thick layer. Next, the sample is soft baked on a hot plate for 60 seconds at a temperature of 90⁰ C. Photolithography is performed using Karl Suss contact lithography system. The dose required for AZ 1813 is 120 mJ/cm², while the contact lithography system provides a dose of around 14 mJ/cm², so the duration for exposure is 8.5 seconds. After exposure, the resist is developed in AZ 917 MIF developer for 30 seconds to create the copper nodule pattern (blue pattern in the mask layout of Figure 4.2).

After the lithography step, the sample is mounted in a carrier Si wafer and is put it in the DRIE machine. The Ge-on-Si sample is attached to the carrier wafer with the help of a small amount of AZ 1813 photoresist. A small drop of the photoresist is put on top of the carrier wafer, and the sample is placed on top of the resist droplet. Then the resist is
dried to attach the sample. The resist also works as an epoxy between the carrier wafer and the sample, which is very important to keep the sample at the DRIE system substrate temperature of 20° C. Highly selective etch ratio between Si/Ge and masking photoresist layer is only achieved when the sample is at the same temperature as the DRIE substrate. With the above mentioned conditions, the etch rate in DRIE is found to be ~2.5 μm/min for Ge and ~5 μm/min for Si. As a result, a 4 minute etch of the Ge-on-Si sample creates ~15 μm deep copper nodule trenches (Figure 4.5).

4.2.2 Copper Nodule Fabrication

After the trench etch, the copper nodules are fabricated. The fabrication process can be divided into three steps:

1. A copper seed layer deposition by sputtering to define the area of the electroplating.
2. An electrolytic copper plating to fill up the trenches.

3. A CMP process to polish the excess copper for forming the nodule.

These three steps are discussed in detail in Sections 4.2.2.1 to 4.2.2.3. A schematic of the process is shown in Figure 4.6.

4.2.2.1 Sputter Deposition of Copper Electroplating Seed Layer

After etching the copper nodule trenches, sputtering is done (by Oerlikon PE 2400 sputter deposition system) in order to deposit the copper seed layer for the electroplating step. A thin layer of titanium (Ti) is deposited before the copper layer in order to promote adhesion. During the sputter deposition, a ~200 nm layer of titanium is deposited first, followed by a ~1000 nm layer of copper. The Ge-on-Si sample is partially covered during the sputtering step in order to protect the area on the chip, where the waveguides will be fabricated later. Small bare Si wafer pieces are used to cover the chip in order to protect the waveguide portion of the chip from the seed layer deposition, which enables the sample to go through the selective CMP process. The selective CMP process is important to reduce the damage of the Ge layer on the waveguide sample, which is introduced by the abrasive CMP slurry particles. Ge layer damage by the CMP slurries will be discussed in detail in Section 4.2.2.3. An image of the selectively sputtered Cu/Ti seed layer is shown in Figure 4.7.
Figure 4.6: Schematic process flow of the copper nodule fabrication.
4.2.2.2 Copper Electroplating

Electroplating is used in order to fill up the nodule trenches. Electroplating is a commonly used technique to deposit thick layers of metal. In the OQP process, electrolytic copper plating is used to fill up the 15 μm deep copper nodule trenches [40], [41]. Electrolytic plating is an electrochemical reactive process, which takes place under the influence of electric current. During the electroplating process, the Ge-on-Si sample (with patterned seed layer) is connected to the negative bias as the cathode, and a copper metal chuck is connected to the positive bias as the anode. The intended waveguide region on the Ge-on-Si sample is covered with Kapton tape in order to provide a barrier layer for copper accumulation (shown in Figure 4.8), because both Ge and Si have finite resistivity. It allows to reduce the CMP process time, since only the
area around the nodules on the chip is required to be polished. Also, the Ge layer on the chip is protected from any copper accumulation.

During the electroplating process, both the cathode and the anode are immersed in a conductive plating solution containing cupric ions. With sufficient current flow from anode to cathode, the following reactions take place:

1. At cathode Cu$^{2+}$ is reduced to Cu
   \[
   Cu^{2+} + 2e^- \rightarrow Cu .
   \]

2. At anode Cu produces Cu$^{2+}$ ions
   \[
   Cu \rightarrow Cu^{2+} + 2e^- .
   \]

The flow of positive Cu$^{2+}$ ions through the electroplating solution enables the continuous flow of current. The electroplating process to fill up the trenches is similar to standard Quilt Packaging plating process [40], [42]. The detail of the copper electroplating process is described in Appendix C.

Figure 4.8: Kapton tape covering the waveguide area of the chip for selective copper electroplating.
4.2.2.3 Chemical Mechanical Polishing

During the electroplating process, the area on the chip surrounding the copper nodules also accumulates copper. As a result, excess copper is required to be removed to realize the copper nodules. Chemical mechanical polishing (CMP) is a widely used process in semiconductor fabrication industry to planarize and smooth surfaces with the combination of chemical and mechanical forces [43]. It is used widely in the ultra-large-scale-integrated (ULSI) circuits to remove films, planarize wafers and construct damascene interconnects. As the name suggests, CMP uses mechanical abrasion combined with chemical reaction in order to polish the surface. CMP is carried out by using slurries, consisting of fine abrasive particles suspended in an aqueous media containing chemical reagents. During the CMP process, higher areas on the wafer are removed without affecting lower areas. As a result, the wafer becomes isotropic and planar. In the CMP process, a rotating carrier holds the wafer, which is pressed face-down by back pressure. Then, the wafer is brought in contact with a rotating platen holding the polishing pad, which is shown in Figure 4.9 [43]. CMP combines both mechanical and chemical actions. The purpose of using chemical reagents in slurries is to soften the material and make the mechanical abrasion easier. The CMP instrument used in the process is from Logitech. The slurry used in initial tests is Ultra-Sol®A-15 from Eminess. The slurry is first fully mixed with DI water in 1:3 ratio for 30 minutes (using a magnetic stirrer). Then, hydrogen peroxide (H₂O₂) is added to the slurry mix at the volume ratio of H₂O₂: slurry mix = 1: 6, and is mixed for another 15 minutes.
During the CMP process with the Ultra-Sol®A-15 slurry, the abrasive slurry particles polish away the top Ge layer fully. To solve the problem, the CMP process is modified with an alternative slurry called COPPEREADY® CP 72B (Air Products). COPPEREADY® CP 72B is engineered specifically to remove trace metals, organics and particle from copper, tantalum/tantalum nitride etc. during the post-CMP cleaning of the CMP pads. Although the damage is reduced on the Ge layer using COPPEREADY® CP 72B, the Ge layer still gets scratches during the polishing. An image of the damaged surface is shown in Figure 4.11. In order to solve the problem, the CMP process is modified in two ways. Firstly, a new type of polishing pad is introduced (SPM3100 from Eminess), which is generally used as a CMP finishing pad. The pad uses poromeric
technology, which has been developed for silicon final stage polishing. Also, SPM3100 pad has been used with a variety of other materials, where surface finish is defined by haze, micro-scratches, and light point defects [44]. Secondly, the waveguide area on the Ge-on-Si sample is covered with Kapton tape during the polishing, which protects the surface from getting damaged. However, during the CMP process the tape is sometimes peeled away due to the friction with the CMP pad. As a result, the CMP process is required to be watched carefully, so that the process can be stopped, if required in order to prevent Ge layer damage.

Next, a careful CMP process including the above modifications is done to get a sample with an unscratched and undamaged waveguide region. In Figure 4.12, the unscratched Ge-on-Si sample (in the waveguide region) is shown. The sample is used to fabricate Ge-on-Si waveguides in the following step.

Figure 4.10: A CMP process in progress.
Figure 4.11: Ge layer damaged in the CMP process.

Figure 4.12. Unscratched Ge layer with improved CMP process.
4.2.3 Germanium Etch to Define the Waveguide

In the waveguide fabrication step, reactive ion etching (RIE) is used to etch the Ge layer from the top surface of the Ge-on-Si sample. In this step, double trench Ge-on-Si waveguides are fabricated on the CMP polished Ge-on-Si sample. The optimized recipe to etch Ge is shown in Table 4.1. In order to pattern the waveguides, AZ 1813 photoresist is used in this step, with the same lithography recipe discussed in Section 4.2.1. The optimized etch recipe (Table 4.1) is used to etch Ge from the top of the Ge-on-Si sample. An 80 second etch is done in order to get 4 μm high double trench Ge-on-Si waveguides. The RIE process shows very good selectivity for Ge over Si, with an etch ratio of around 10:1 [45]. An array of Ge-on-Si waveguides (each 50 μm wide and 4 μm high) prepared by RIE is shown in Figure 4.13.

| TABLE 4.1 |
| GE ETCH RECIPE FOR RIE [45] |

<table>
<thead>
<tr>
<th>Pressure</th>
<th>100 m Torr</th>
</tr>
</thead>
<tbody>
<tr>
<td>RF Power</td>
<td>200 W</td>
</tr>
<tr>
<td>DC Bias</td>
<td>280 V</td>
</tr>
<tr>
<td>Gas</td>
<td>CF₄ - 50 sccm, O₂ -10 sccm</td>
</tr>
<tr>
<td>Etch Rate</td>
<td>3 μm/min</td>
</tr>
</tbody>
</table>
4.2.4 DRIE Separation and Backside Thinning

After fabricating the Ge-on-Si waveguides, a separation etch is required to release the two parts of the OQP sample. Also, the extension of the copper alignment nodule is released in this step. DRIE is used to do the etch process. Thick photoresist AZ4620 is used to form the protection mask for the DRIE separation. A Ge-on-Si sample, which is lithographically patterned with AZ 4620 resist, is shown in Figure 4.14. The measured etch rates of DRIE are ~3 μm/min for Ge and ~5 μm/min for Si. In the DRIE step, the waveguide facets are simultaneously prepared with the release of the copper nodules. The etch is done for 65 minutes in order to make a deep separation trench in the Ge-on-Si sample (~325 μm). The sample is then cleaned with acetone and
isopropanol in order to remove the remaining photoresist. Next, any remaining photoresist residue is removed by submerging the samples in AZ EBR solvent for at least 2 hours. Next, back side grinding is performed (Disco grinder) in order to release the two single-sided OQP Ge-on-Si samples. The grinding process is done in order to reduce the DRIE process time. The process is done for ~225 \( \mu m \), which produces the final two single-sided OQP samples of ~300 \( \mu m \) thickness (original Ge-on-Si sample thickness is ~525 \( \mu m \)). The DRIE etched Ge-on-Si sample is shown in Figure 4.15.
4.3 Alignment of the Waveguide Chips via Copper Nodules

After DRIE separation the single sided OQP chips are aligned via released copper nodules. 'Finetech fineplacer' system is used for the alignment. The nodules are connected in an interdigitated fashion in order to align the waveguides. After alignment, the nodules are pushed in order to reduce the inter-chip distance. The initial proof-of-concept OQP structure (with a bare Si sample) is fabricated following the fabrication steps, which are described in Section 4.2. The Si OQP sample has an inter-chip distance of \(~10 \mu m\) (Figure 4.16). In the Si OQP sample, the copper nodules are protruded 50 \(\mu m\) from the side face of the chip, and there are 5 nodules in each nodule set (each individual nodule is 20 \(\mu m\) wide). The chip-to-chip distance can only be reduced to \(~10 \mu m\) with this design, without damaging the copper nodules (\(~10\) dB expected coupling loss for QCL to Ge-on-Si coupling, and \(~8\) dB expected loss for Ge-on-Si to Ge-on-Si
coupling). The force, which is used in order to reduce the inter-chip distance further, breaks the nodules in this case. As a result, in order to reduce the inter-chip distance, the nodules are required to be more robust and less protruded.

A new design is proposed to reduce the inter-chip distance, where the copper nodules are protruded only 20 μm from the side face. Also, in order to increase the robustness, the individual nodules are designed to be 50 μm wide. The goal of the design is to make the copper nodules more resistant to the force to be used for reducing the inter-chip gap in order to reduce the optical coupling loss.

Next, a new OQP Ge-on-Si device is fabricated with the improved design. A single sided Ge-on-Si waveguide chip, which is fabricated with the new design, is shown in Figure 4.17. Copper nodules show great stability during the DRIE process, with 50.2±0.7 μm in width (designed as 50 μm), and with 52.9±0.7 μm spacing in between them (designed as 54 μm). Then, two single sided Ge-on-Si chips are aligned via copper
nodules. The new OQP chip has inter-chip distance of 4.6±1.1 μm, and lateral misalignment of 920±153 nm in between the waveguide arrays (Figure 4.18). The inter-chip gap seems to get increased from the Si substrate top to the Ge layer top (as seen in Figure 4.18). Some possible explanation for this could be:

1. The substrate thickness may not be uniform after CMP.
2. The DRIE process could introduce slight slope in the etched face, rather than making a 90° vertical etch.
3. The force exerted to reduce the inter-chip gap can push the chips upward at their faces.

An improved approach with sputter deposited copper nodule is taken in the second generation OQP fabrication process to minimize these effects and decrease the inter-chip gap.

4.4 Second Generation OQP Process

The first OQP Ge-on-Si waveguide sample has inter-chip distance of 4.6±1.1 μm, and lateral misalignment of 920±153 nm (Figure 4.18). This should reduce the chip-to-chip optical coupling loss to ~3.5 dB (expected), which is a good number for a 'butt coupled' optical device (as discussed in Chapter 3). However, the fabrication process requires some improvement, since there is risk of surface damage during the CMP process. The Kapton tape barrier layer, which is placed on the waveguide region in order to protect the CMP damage, loses its adhesion quality gradually in contact with the
Figure 4.17: (a) Single-sided OQP Ge-on-Si waveguide chip, (b) the SEM of the copper nodules, and (c) a single waveguide.

Figure 4.18: Ge-on-Si waveguide chips aligned via OQP.
chemical slurry. If the tape is peeled off during the CMP, the Ge layer could be damaged. As a result, in order to achieve a high yield fabrication process, it is important to eliminate the CMP step. An alternative approach to fabricate the copper nodules is discussed in this section, which eliminates the CMP step from the fabrication process.

4.4.1 Copper Nodule Fabrication by Sputter Deposition

In the new approach of eliminating the CMP process from the fabrication steps, copper nodules are fabricated via sputter deposition. Copper nodule fabrication via sputtering is inspired from metal "lift-off" process [46], which is widely used in micro-fabrication industry. Lift-off can support structures from nanometer to centimeter scale. It is a simple method for patterning deposited films, which are difficult to dry etch. Typically a metallic film is blanket-deposited on all over the substrate surface, which covers a patterned photoresist layer underneath. The sample is then submerged into a solvent, which removes the photoresist layer. As a result, the film which has been deposited directly on the substrate, creates an inverted pattern of the resist layer [47]. The new fabrication scheme is illustrated step-by-step in Figure 4.19. Although, both sputtering and electron-beam evaporation can be used for depositing the copper, sputtering is preferred due to the higher deposition rate between the two available deposition systems (~50 nm/min for the sputtering and ~10 nm/min for the evaporator). Electron-beam evaporation is particularly preferred in metal lift-off technology as it can produce discontinuous film on the lithographically patterned layer (with no side wall deposition). In our case, the copper nodule width and height ratio is
Figure 4.19: Illustration of Cu nodule fabrication by sputter deposition.
5:1. As a result, we do not observe any significant side-wall deposition (nodules do not have higher edges) in the fabricated copper nodules (Shown in Figure 4.20(a)). The fabrication steps of the copper nodules via sputter deposition are described below:

1. A thick (~22 μm) AZ 4620 photoresist layer is patterned for the copper nodules by contact lithography. The resist height is achieved by spinning the resist twice. In conventional lift-off process, it is recommended to have the 1:3 thickness ratio between the deposited film and the sacrificial resist layer [47]. Here, the nodule voids are designed as 10 μm deep. So, the ratio criterion is fulfilled (10 μm: 32 μm = 1:3.2; shown in Figure 4.20).

2. 10 μm deep trenches are etched by DRIE.

3. Ti is sputtered for 10 minutes (~0.5 μm), and then Cu is sputtered for 130 minutes (~7 μm).

4. The sample is submerged in acetone for 2 hours in order to remove the sacrificial resist layer.

The optical micrograph of the fabricated copper nodules via sputter deposition is shown in Figure 4.20(b). The copper nodules show consistency in geometry, and the

Figure 4.20: (a) SEM of the sputter deposited copper nodules, and (b) Ge-on-Si sample after copper deposition and lift-off.
measured height of the nodules are \(\sim 7.5 \mu m\) (designed as 10 \(\mu m\)). Also, the top surface of the sample is free of any scratches, which supports our motivation of modifying the conventional copper nodule fabrication process.

4.4.2 OQP Sample with Sputter Deposited Copper Nodules

Next, another OQP Ge-on-Si sample is fabricated, where the copper nodules are fabricated by sputtering. Also, the Ge-on-Si waveguides are bent in this sample in order to address an optical measurement issue, which will be discussed in Chapter 5. In the sample, the top Ge surface is free of any damage. As a result, the waveguides are scratch free, which is shown in Figure 4.21. An array of 50 \(\mu m\) wide waveguides is

![Figure 4.21: Ge-on-Si waveguides fabricated with sputter fabricated Cu nodule sample.](image-url)
Figure 4.22: OQP sample after DRIE separation etch (before back side grinding).

fabricated. There are 4 waveguides in the array. The 50 μm wide dimension is chosen in order increase the lateral modal overlap during coupling (multimode propagation). In Figure 4.22, the sample after the separation etch is shown. The aligned Ge-on-Si OQP sample (with sputter deposited copper nodules) is shown in Figure 4.23.

In the OQP sample, where copper nodules are fabricated by sputtering, the inter-chip gap is reduced more. The inter-chip distance is 1.4±0.3 μm in the new OQP sample [10]. According to the FDTD simulation, which is discussed in Chapter 3, the expected coupling loss for the sample is ~6.5 dB. The loss is lower than that of the conventional butt coupling loss. The vertical mismatch between the aligned chips is investigated with an optical microscope. The microscope with a numerical aperture of
Figure 4.23: OQP sample with sputter deposited copper nodules.

0.9 and a 100 times objective zoom has a depth of focus of \( \sim 0.7 \, \mu m \). The aligned chip edges are easily visible in the micrograph taken with this depth of focus (Figure 4.24). As a result, the vertical misalignment should be less than 0.7 \( \mu m \). Additionally, horn-shaped waveguides are implemented in the second chip, which should reduce the coupling loss more. The horn geometry used in the newly fabricated device does not follow the simulation results (Chapter 3), rather it is similar to the previously demonstrated horn waveguide geometry that has been used in a MIR butt coupling [15]. The horn has two
sections: (a) a 100 μm wide and 350 μm long rectangular section at the inlet of the waveguide, and (b) a 150 μm long tapered section to reduce the waveguide width from 100 μm to 50 μm. This specific horn geometry is designed to be suitable for the OQP sample with cleaved waveguide facets.

![Image of waveguide chips]

Figure 4.24: Optical micrograph of the aligned waveguide chips.

4.5 DRIE Fabrication of Waveguide Facet

In the OQP fabrication technique, the Ge-on-Si waveguide facets are prepared by DRIE process. In the conventional QCL fabrication process, the waveguide facets are fabricated by cleaving [48]. However, etched facet QCLs have also been reported for both MIR and THz ranges [49], [50]. In THz QCL, the emission power could even be higher from the etched facet than that of the cleaved facet [49]. But, the mirror loss is higher in the etched facet, since the facet has more irregularities. If the irregularities
(due to the etching) are smaller in size compared to the emission wavelength, QCL facets can also be fabricated by etching. A Ge-on-Si waveguide facet prepared by DRIE is shown in Figure 4.25. The SEM micrograph shows that the etched sidewall has irregularities lower than 0.5 μm in size that is smaller than the MIR wavelength (λ = 8 μm) used in the MEEP simulations. So, if a similar quality etches can be performed in a QCL sample, the OQP process will be compatible with QCL chips.

Figure 4.25: SEM micrographs of (a) a DRIE fabricated Ge-on-Si waveguide facet, and (b) a zoomed view of the facet showing the irregularities formed during the etch.

4.6 Conclusion

OQP Ge-on-Si sample has been fabricated with the minimum inter-chip distance of ~1.4 μm. The expected coupling loss for the sample is ~6.5 dB, which is lower than that of the conventional butt coupling loss. The coupling loss is reduced more when the inter-chip gap is around the half of the laser emission wavelength. The lowest coupling loss is achieved when the waveguides touch each other at their facets (zero inter-chip distance). Also, expensive QCL chips can now be used in OQP process, since the surface
damaging CMP step is eliminated from the fabrication process. Next, the coupling loss associated with the fabricated Ge-on-Si OQP is measured, which will be discussed in Chapter 5.
5.1 Introduction

In this chapter, optical measurements are done to evaluate OQP coupling loss performance across an array of waveguides. In order to measure the optical coupling loss of the butt-coupled waveguides, a Fourier transform infrared (FTIR) spectroscopy system with a mid-infrared 'globar' source is used at first. The globar, however, lacked enough power to be used in the measurement. We therefore used a higher power quantum cascade laser as the source, which proved to be appropriate for these measurements. In the optical measurement with QCL, the OQP sample with an inter-chip distance of $1.4\pm0.3 \, \mu m$ is used (the same OQP sample with sputter deposited copper nodules discussed in Chapter 4). In the optical measurement scheme the MIR light is focused to one of the Ge-on-Si waveguide facets, and the light coming out from the other waveguide is measured to determine the optical coupling loss.

5.2 Optical Coupling Loss Measurement with Quantum Cascade Laser

The OQP coupling loss is measured by comparing optical transmission through two OQP coupled waveguides to that of a reference sample. The reference sample is an
undivided Ge-on-Si waveguide of the same length and shape (except the horn structure) as the combined OQP waveguides. In the optical measurement setup (shown in Figure 5.1 and Figure 5.2), the output of a $\lambda=8.4 \, \mu m$ QCL is focused to the input facet of the first chip. The optical power of the QCL is 300 mW. ZnSe plano-convex lenses (RMI Infrared) are used to focus the QCL beam to the facet of the Ge-on-Si waveguide chip. ZnSe lenses offer high transmission for the spectral range of 0.6-16 $\mu m$, and are available with broadband anti-reflection coating (on both surfaces of the lens), which is optimized for 8-12 $\mu m$ wavelength range. A vanadium-oxide (VoX) thermal imaging camera (Seek Compact from Seek Thermal, Inc) is used to image the QCL beam during preliminary alignment with the Ge-on-Si waveguide. After the initial alignment, the OQP sample is translated using a 3-dimensional stage in order to maximize the input light. Light exiting from the second chip is measured with a liquid nitrogen cooled photoconductive mercury-cadmium-telluride (MCT) detector with a ZnSe window (from Teledyne Judson technologies). The detector has high sensitivity over a broad spectral band of 2-18 $\mu m$. The MCT is moved using another 3-dimensional translation stage to detect maximum optical signal. To ensure that only coupled light is measured at the output, the waveguides incorporate a 90° bend such that the output is normal to the input (Figure 5.3), as is done in modular MIR optical waveguides [2]. The approach blocks the MIR light, which is transmitted through the Si substrate, to reach the MCT detector. To further eliminate the light transmitted through the Si substrate, a razor blade partially covers the bottom half of the light exiting second chip facet. Also, black cardboard walls are placed on both sides of the exiting beam path in order to block any
QCL light reflected from the lab equipments to the MCT, which is shown in Figure 5.1. The laser is modulated at 500 Hz, and the output from the MCT is fed to a lock-in amplifier to increase the sensitivity of the measurement. The MCT signal measured from the lock-in amplifier is kept below 100 mV in order to avoid any damage to the detector due to the high QCL power. Each measurement is repeated by changing the translation direction of the MCT, and the average of the reading from the lock-in amplifier is considered as the measured signal. Each waveguide has an identical bend structure with a radius of curvature = 250 $\mu$m. According to the MEEP simulations, the waveguide bend loss is less than 3% for the fabricated 90° bend structure. The waveguide bend loss is normalized in the measurement since both the reference and the OQP sample have identical bend radii. Also, both the OQP and reference samples are expected to have the same insertion loss, propagation loss with length, and reflection loss at the output facet. The reference sample does not have the horn structure in order to measure the total OQP loss. Therefore, normalizing output loss in both the reference and OQP samples to the loss of the shortest reference waveguide ($\ell= 9.6$ mm) yields the following expressions for normalized loss in dB:

\begin{align*}
L_{\text{Ref}} &= \alpha \ell & (5.1) \\
L_{\text{OQP}} &= \alpha \ell + L_c & (5.2)
\end{align*}

where $L_{\text{Ref}}$ is the normalized reference sample loss, $L_{\text{OQP}}$ is the normalized OQP loss, $L_c$ is the OQP optical coupling loss, $\alpha$ is the propagation loss coefficient, and $\ell$ is the waveguide length. Therefore, comparing measured loss (in dB) versus waveguide length
Figure 5.1: Coupling loss measurement scheme of Ge-on-Si OQP sample with QCL mid-infrared source.

Figure 5.2: Optical setup for OQP coupling loss measurement.
will yield waveguide propagation loss (slope) and OQP coupling loss (difference between reference and OQP loss for same waveguide length). From Figure 5.4, OQP coupling loss is measured to be 9.0±0.1 dB. To further reduce coupling loss, we filled the OQP inter-chip gap with high-index and MIR transparent As$_2$S$_3$ chalcogenide glass ($n=2.4$ at $\lambda=8.4$ μm). As$_2$S$_3$ powder (Alfa Aesar) is dissolved in anhydrous propylamine solvent (>99.0%, Sigma-Aldrich) at a concentration of 0.2 g/ml [34]. The solution is then placed in the OQP inter-chip gap as a droplet, and dried in nitrogen for one hour, forming solid As$_2$S$_3$ glass. An optical micrograph of the As$_2$S$_3$ glass droplet on the Ge-on-Si OQP sample is shown in Figure 5.5. The coupling loss measurement with the index-matching material is shown in Figure 5.4 (dashed line). The coupling loss is reduced to 4.1±0.3 dB, which is the lowest loss with MIR butt-coupling to our knowledge [10].
Figure 5.4: Normalized optical transmission for three waveguides in a waveguide array; reference (no inter-chip coupling) in straight, OQP coupling in dotted, and OQP with index-matching material in dashed lines.

Figure 5.5: Ge-on-Si OQP sample with index matching As$_2$S$_3$. 

As$_2$S$_3$ Glass
Propagation loss is measured to be 2.9 dB/cm, 3.7 dB/cm and 0.6 dB/cm for the OQP, reference samples, and index-matched OQP (the waveguide loss with the index-matched OQP is measured as 4.9±0.2 dB), respectively, similar to what is expected for Ge-on-Si [10], [15]. The lower loss of the index-matched sample can be attributed to the reduced interface loss due to the formation of an As$_2$S$_3$ cladding on the top and the sides of the waveguides [51]. The As$_2$S$_3$ cladding reduces the surface roughness loss of the Ge-on-Si waveguides. The surface roughness is created during the reactive ion etching process. Similar example of scattering loss reduction is found in the work of Seibert et al., where oxygen-enhanced nonselective wet thermal oxidation is used to smooth the sidewall roughness in high-index-contrast AlGaAs heterostructure ridge waveguides [52].

5.3 Conclusion

MIR coupling loss between two passive OQP Ge-on-Si rib waveguide arrays is measured with a QCL as the optical source. OQP inter-chip coupling loss was measured to be 9.0±0.1 dB when the inter-chip gap was in air and 4.1±0.3 dB when filled with As$_2$S$_3$ glass [10]. These results represent lower loss than previously reported chip-to-chip MIR optical coupling via butt-coupling [2], [15], fiber coupling (as low as ~10 dB [6], [53]), and grating coupling (tens of dBs loss [54]). Additionally, OQP allows simultaneous optical coupling of waveguide arrays using the copper nodules, which is cheaper and simpler to fabricate than other waveguide array coupling techniques. Currently available semiconductor waveguide array coupling techniques are expensive compared to OQP,
not compatible in MIR, or require each interconnect of the array to be made individually [8], [12]. OQP copper nodules are design to simultaneously align waveguide arrays while maintaining uniform coupling loss throughout the array. The OQP coupling loss characteristics is compared with the other MIR coupling techniques in Table 5.1:

**TABLE 5.1**

**COMPARISON OF COUPLING CHARACTERISTICS AMONG THE MIR OPTICAL COUPLING TECHNIQUES**

<table>
<thead>
<tr>
<th></th>
<th>Grating coupling</th>
<th>Fiber coupling</th>
<th>Butt coupling</th>
<th>OQP</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Waveguide Array Coupling</strong></td>
<td>Possible, but coupling loss is high [55]</td>
<td>Possible, but the alignment is hard [56]</td>
<td>Theoretically possible, but technically difficult and not yet demonstrated.</td>
<td>Demonstrated with OQP for an array of 3 waveguides with a standard deviation of 0.3 dB [10]</td>
</tr>
</tbody>
</table>
CHAPTER 6:
FUTURE WORK AND CONCLUSION

6.1 Introduction

In this dissertation, OQP technique is demonstrated as an MIR optical integration technique for realizing on-chip modular systems in future. In this chapter, the future work with the OQP technique will be presented with the summary of OQP research progress.

6.2 Future Work

OQP technique is capable of coupling QCL directly to the Ge-on-Si waveguide platform. QCLs are ideal devices for MIR sensing/imaging. However, widely tunable QCLs require external cavity tuning, and are thus susceptible to mode-hopping instabilities and mechanical failure, which severely limits their performance. These issues can be solved by developing QCL arrays where each device in the array has a unique output wavelength, which is developed by Pendar Technologies (Figure 6.1). To maintain high signal-to-background contrast with small trace samples on substrates, high resolution imaging is required. In an imaging system, however, each of the lasers in the array must follow the same beam path, which is not possible from laser waveguide arrays. OQP develops a new micro-fabrication technique, which can be used to combine
the light out from MIR lasers array into an inexpensive silicon based chip. The light can then be used for imaging of explosives in small quantities, or sensing chemical and biological analytes. With the improved approach of fabricating copper nodules via sputter deposition, potentially destructive surface polishing is avoided in OQP fabrication process. This improved technique enables OQP to be implemented with InP QCL substrates. So, a QCL array chip will be coupled with a Ge-on-Si waveguide array via OQP in future. The scheme is illustrated in Figure 6.2.

Figure 6.1: A tunable QCL array from Pendar Technologies [59].
6.3 Summary and Conclusion

In this Section we will summarize the progress in OQP research described in this dissertation.

In Chapter 2, an eigenmode expansion technique is used to develop a mathematical model for chip-to-chip optical coupling via OQP. The mathematical model is then used to gain insight into the expected performance and limitations of OQP. The modeling results suggest that OQP needs to overcome the challenges of precise lateral, vertical, and axial alignment for successful heterogeneous coupling between QCL and passive semiconductor waveguides.

Next, simulations are performed in Chapter 3 in order to determine coupling loss as a function of lateral and axial alignment between QCL and Ge-on-Si waveguide structures. Initial simulation results suggest good feasibility for OQP chip-to-chip optical
coupling. If submicron precision alignment can be implemented with an inter-chip distance of lower than or around 4 \( \mu m \) (for 8 \( \mu m \) wavelength), OQP offer great prospect in wide-bandwidth, highly efficient optical coupling. Also, the coupling loss can be further reduced by applying horn geometries in the waveguide structures and by filling the inter-chip gap with high-index and MIR transparent As\(_{2}\)S\(_{3}\) chalcogenide glass.

Chapter 4 describes the detailed fabrication process for OQP coupling between two separate Ge-on-Si waveguide chips. The OQP fabrication process on Ge-on-Si is optimized. Waveguides of separate substrates have been aligned with sub-micron accuracy by protruding, lithographically defined interdigitated copper nodules, placed on the side of the chip. A new approach to fabricate copper nodules by sputter deposition is proposed and realized. This reduces the complexity of the OQP fabrication process and makes the process suitable for III-V material processing (e.g., QCL material). Also, it makes OQP a perfect candidate to combine Si/Ge and III-V materials into a single heterogeneous platform.

In Chapter 5, OQP coupling loss measurement technique and the measurement results are presented in detail. In the optical measurement of OQP with a QCL, the Ge-on-Si OQP sample with an inter-chip distance of 1.4±0.3 \( \mu m \) is used. OQP coupling loss is measured to be 9.0±0.1 dB, which further reduces to 4.1±0.3 dB when an MIR transparent As\(_{2}\)S\(_{3}\) chalcogenide glass is used to fill the inter-chip gap [34].

The OQP coupling loss is lower than previously reported chip-to-chip MIR optical coupling via butt-coupling [2], [15], fiber coupling (as low as ~10 dB [6], [53]), and grating coupling (tens of dBS loss [54]). Also, OQP allows simultaneous optical coupling
of waveguide arrays, which is cheaper and simpler to fabricate than other waveguide array coupling techniques. Currently available waveguide array coupling techniques are expensive compared to OQP, not compatible in MIR, or require each interconnect of the array to be made individually [8], [12]. OQP copper nodules are design to simultaneously align waveguide arrays while maintaining uniform coupling loss throughout the array. In conventional butt-coupling, the manual alignment is done in order to allow maximum light to be coupled between the aligned waveguides. Since there is no permanent mechanical bond between the waveguide chips, the coupling loss varies from one experiment to another. On the other hand, OQP reduces the non-uniformity in coupling loss with the permanent alignment between the waveguide arrays via copper nodules. In future, the coupling loss could be reduced further by optimizing the horn geometry. The horn structure can be investigated with the change of horn-head and the tapered section dimensions and shapes in order to reduce the coupling loss (e.g., taper length variation or a s-bend in the taper). The lateral misalignment accuracy can be increased with the use of stepper lithography system. Indiana Integrated Circuits, LLC, has fabricated electrical QP chips with ~0.1 \( \mu m \) lateral misalignment via copper nodules fabricated with stepper lithography in an unpublished work. The lateral misalignment between the OQP chip is approximately the same as the measured standard deviation of the copper nodule width (as described in Chapter 4). As a result, fabricated copper nodule dimension accuracy can reduce the lateral misalignment. Stepper lithography will increase the accuracy of the fabricated copper nodule dimensions. Also, the inter-chip gap can be reduced further with the improved lithography technique (the goal is to
reduce the inter-chip gap to 0). As a result, OQP would be compatible with the telecom laser optical coupling with the reduced misalignment between the waveguide arrays. All these results and future prospects establish OQP as a low-loss, inexpensive technique for MIR chip-to-chip waveguide array coupling.
APPENDIX A:

EIGENMODE EXPANSION

A.1 Wave Equation for TM Propagation Magnetic Field

If $E$, $H$, $D$ and $B$ are the phasor forms of the electric field, the magnetic field, the electric flux density, and magnetic flux density respectively, the phasor form of Maxwell's equation can be expressed as following:

\[
\nabla \times E = -j \omega B = j \omega \mu_0 H, \tag{A.1}
\]

\[
\nabla \times H = -j \omega D = j \omega \varepsilon_0 \varepsilon_r H, \tag{A.2}
\]

\[
\nabla \cdot H = 0, \tag{A.3}
\]

\[
\nabla \cdot (\varepsilon_r E) = 0. \tag{A.4}
\]

The assumptions made in equation (A.1) to (A.4) are $\mu_0 = 1$, and $\rho = 0$. Now, vector rotation operator $\nabla \times$ is applied to equation (A.2) to get:

\[
\nabla \times (\nabla \times H) = j \omega \varepsilon_0 \nabla \times (\varepsilon_r E). \]

So, \[
\nabla \cdot (\nabla \cdot H) - \nabla^2 H = j \omega \varepsilon_0 (\nabla \varepsilon_r \times E + \varepsilon_r \nabla \times E)
\]

\[
= j \omega \varepsilon_0 (\nabla \varepsilon_r \times E) + j \omega \varepsilon_0 \varepsilon_r (-j \omega \mu_0 H))
\]

\[
= j \omega \varepsilon_0 (\nabla \varepsilon_r \times E) + k_0^2 \varepsilon_r. \tag{A.5}
\]

where \[
k_0^2 = \omega^2 \mu_0 \varepsilon_0
\]
Now, using

\[ E = \frac{1}{j \omega \varepsilon_0 \varepsilon_r} \nabla \times H \]

and equation (A.2) and (A.3), the following relation is obtained:

\[ \nabla^2 H + \frac{\nabla \varepsilon_r}{\varepsilon_r} \times (\nabla \times H) + k_0^2 \varepsilon_r H = 0, \]

or

\[ \nabla^2 H + \frac{\nabla \varepsilon_r}{\varepsilon_r} \times (\nabla \times H) + k^2 H = 0, \]  \hspace{1cm} (A.6)

where \( k = k_0 n = k_0 \sqrt{\varepsilon_r} \).

In our analysis, relative permittivity \((\varepsilon_r)\) is constant for a specific medium. Thus, the wave equation becomes:

\[ \nabla^2 H + k^2 H = 0. \]  \hspace{1cm} (A.7)

Equation (A.7) is called the Helmholtz equation.
A.2 Maxwell’s Equation and Helmholtz Equation

In electromagnetism, the electric field $\mathbf{E}$, the magnetic field $\mathbf{H}$, the electric flux density $\mathbf{D}$, and the magnetic flux density $\mathbf{B}$ are related to each other by the following equations:

$$\mathbf{D} = \varepsilon \mathbf{E},$$  \hspace{1cm}  (A.8)

$$\mathbf{B} = \mu \mathbf{H}.$$  \hspace{1cm}  (A.9)

Here, $\varepsilon$ is the permittivity of the medium and $\mu$ is the permeability of the medium, and they are defined as:

$$\varepsilon = \varepsilon_0 \varepsilon_r,$$  \hspace{1cm}  (A.10)

$$\mu = \mu_0 \mu_r,$$  \hspace{1cm}  (A.11)

where $\varepsilon_0$, $\mu_0$, $\varepsilon_r$, and $\mu_r$ are the vacuum permittivity, vacuum permeability, relative permittivity, and relative permeability of the material, respectively. The discussion in this chapter does not involve any magnetic material, so $\mu_r$ will be considered as 1 [19].

According to the Maxwell’s equation, the electromagnetic fields follow the relations:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t},$$  \hspace{1cm}  (A.12)

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J},$$  \hspace{1cm}  (A.13)

where $\mathbf{J}$ is current density, and is related to the electric field by the equation $\mathbf{J} = \sigma \mathbf{E}$ ($\sigma$ is electrical conductivity). Since, any arbitrary vector $\mathbf{Z}$ follows the relation $\nabla \cdot (\nabla \times \mathbf{Z}) = 0$, the following two relations can be derived from equation (A.12) and (A.13) [19]:
\[ \nabla \cdot B = 0, \quad (A.14) \]
\[ \nabla \cdot D = \rho. \quad (A.15) \]

In case of a time harmonic electromagnetic signal, with a single frequency \( \omega \), it is convenient to express the electromagnetic fields in the following form:

\[
Z(r,t) = \text{Re}[Z(r) \exp \{j(\omega t + \theta)\}]
\]
\[
= \text{Re}[Z(r) \exp (j\theta) \exp(j\omega t)]
\]
\[
= \text{Re}[\bar{Z}(r) \exp (j\omega t)], \quad (A.16)
\]

where \( \bar{Z}(r) \) is the phasor representation of \( Z(r,t) \). Following the equation (A.16), the electric field \( E \), electric flux density \( D \), magnetic field \( H \), and magnetic flux density \( B \) can be represented in the phasor form of:

\[
E(r,t) = \text{Re}[\bar{E}(r) \exp (j\omega t)], \quad (A.17)
\]
\[
H(r,t) = \text{Re}[\bar{H}(r) \exp (j\omega t)], \quad (A.18)
\]
\[
D(r,t) = \text{Re}[\bar{D}(r) \exp (j\omega t)], \quad (A.19)
\]
\[
B(r,t) = \text{Re}[\bar{B}(r) \exp (j\omega t)]. \quad (A.20)
\]

For simplicity, phasor notations \( \bar{E}, \bar{H}, \bar{D}, \) and \( \bar{B} \) can be denoted as \( E, H, D \) and \( B \).

Using the phasor form, equation (A.12) to (A.15) can be expressed as the following [19]:

\[
\nabla \times E = -j\omega B = -j\omega \mu_0 H, \quad (A.21)
\]
\[
\nabla \times H = j\omega D = j\omega \varepsilon_0 \varepsilon_r E, \quad (A.22)
\]
\[
\nabla \cdot H = 0, \quad (A.23)
\]
\[
\nabla \cdot (\varepsilon_r E) = 0. \quad (A.24)
\]

The assumptions made in equations (A.21) to (A.24) are: \( \mu_0 = 1 \), and \( \rho = 0 \).
From the phasor form of the Maxwell’s equations, the following Helmholtz equations for electric ($E$) field and magnetic ($H$) field can easily be derived:

$$\nabla^2 E + k^2 E = 0,$$

(A.25)

$$\nabla^2 H + k^2 H = 0,$$

(A.26)

where $k$ is the wavenumber and $\nabla^2$ is a Laplacian defined by:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}.$$  

(A.27)

The detailed derivation is presented in Appendix A.1.

Now, if an optical waveguide with uniform structure along the $z$ direction is considered, the derivative of a spatial harmonic electromagnetic field with respect to $z$ becomes $\frac{\partial}{\partial z} = -j\beta$, where $\beta$ is the propagation constant along the $z$ direction (for the wavenumber $k$). So, the following equation can be written:

$$\frac{\partial^2}{\partial z^2} = -\beta^2.$$  

(A.28)

The ratio between the propagation constant in the medium $\beta$, and the wavenumber in the vacuum $k_0 = \frac{k}{\sqrt{\varepsilon_r}}$ is defined as the effective index:

$$n_{\text{eff}} = \frac{\beta}{k_0}.$$  

(A.29)

The wavelength in vacuum $\lambda_0$, and the $z$ directional component of the wavelength in the propagation medium $\lambda_{\text{eff}}$, are related to the propagation constant $\beta$, by the following equation [19]:

$$\beta = \frac{2\pi}{\lambda_0} n_{\text{eff}} = \frac{2\pi}{\lambda_{\text{eff}}},$$  

(A.30)
where

$$\lambda_{eff} = \frac{\lambda_0}{n_{eff}}.$$  \hspace{1cm} (A.31)

Next, using equation (A.28), the Helmholtz equation for $E$ field can be expressed
as [19]:

$$\nabla^2_{\perp} E + (k^2 - \beta^2)E = 0, \hspace{1cm} (A.32)$$

or

$$\nabla^2_{\perp} E + k_0^2 (\varepsilon_r - n_{eff}^2)E = 0, \hspace{1cm} (A.33)$$

and for $H$ field as:

$$\nabla^2_{\perp} H + (k^2 - \beta^2)H = 0, \hspace{1cm} (A.34)$$

or

$$\nabla^2_{\perp} H + k_0^2 (\varepsilon_r - n_{eff}^2)H = 0, \hspace{1cm} (A.35)$$

where

$$\nabla^2_{\perp} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}.$$  \hspace{1cm} (A.36)

The $H$ field equations (A.34) and (A.35) will be used in the eigenmode analysis of
a TM (transverse magnetic) mode propagation in a waveguide structure in Section 2.2.
A.3 Optical Mode Type

For TM propagation, the following equation for the principle magnetic field component describes the wave propagation:

$$\frac{\partial^2}{\partial x^2} H(x) + k_0^2 (\varepsilon_r(x) - n_{eff}^2) H(x) = 0 \quad (A.37)$$

$$\Rightarrow \frac{\partial^2}{\partial x^2} H(x) + P^2 H(x) = 0, \quad (A.38)$$

where

$$P^2 = k_0^2 (\varepsilon_r(x) - n_{eff}^2) = k_0^2 (n^2 - n_{eff}^2),$$

and

$$n = \text{refractive index of the medium}$$

Now, there could be two cases:

1. If $P^2 > 0$, that means if $n^2 > n_{eff}^2$, then equation

$$\frac{\partial^2}{\partial x^2} H(x) + P^2 H(x) = 0,$$

has a solution in the form:

$$H(x) = A \cos Px + B \sin Px.$$ 

So, the solution of $H(x)$ is oscillatory.

2. If $P^2 < 0$ (i.e., $P = iQ$), that means if $n^2 < n_{eff}^2$, then the field equation becomes:

$$\frac{\partial^2}{\partial x^2} H(x) - Q^2 H(x) = 0.$$ 

The solution of the equation is in the form:

$$H(x) = Ae^{Qx} + Be^{-Qx}.$$ 

So, the solution of $H(x)$ is exponential.
Now, for a three layer slab waveguide with refractive indexes $n_{core}$, $n_{substrate}$ and $n_{cladding}$ (Figure A.1), the mode types are defined by the value of $n_{eff}$. The dependence of mode type on $n_{eff}$ value is shown in Table A.1.

**TABLE A.1**

**MODE TYPE DEPENDENCE ON EFFECTIVE INDEX ($n_{eff}$) VALUE**

<table>
<thead>
<tr>
<th>Effective index relation</th>
<th>$H (x)$ Solution Type</th>
<th>Mode Type</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Core</td>
<td>Substrate</td>
</tr>
<tr>
<td>$n_{core} &gt; n_{eff} &gt; n_{substrate}$</td>
<td>Oscillatory</td>
<td>Exponential</td>
</tr>
<tr>
<td>$&gt; n_{cladding}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$n_{core} &gt; n_{substrate} &gt; n_{eff}$</td>
<td>Oscillatory</td>
<td>Oscillatory</td>
</tr>
<tr>
<td>$&gt; n_{cladding}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$n_{core} &gt; n_{substrate} &gt; n_{cladding}$</td>
<td>Oscillatory</td>
<td>Oscillatory</td>
</tr>
<tr>
<td>$&gt; n_{eff}$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure A.1: A three layer slab waveguide.
Following the above table, the relation between the effective index and the refractive index in the waveguide layers can be used to determine mode type for a specific effective index solution of the eigenmode analysis.
APPENDIX B:
SIMULATION CODES

B.1 A MEEP Code for MIR Transmission from InP QCL to Ge-on-Si Waveguide with Horn

(define-param sx 70)
(define-param sy 18)
(define-param sz 18)
(set! geometry-lattice (make lattice (size sx sy sz)))

(define-param time 20)

(define-param d 3); waveguide substrate separation
(define-param t 4); PML thickness
(define-param break? true)
(define-param dz 0)

(define-param f 0.122) ; center frequency of the pulse
(define-param df 0.014) ; bandwidth of the pulse
(define-param nfreq 100) ; number of frequencies to compute

; all parameters relating to the InP Substrate ridge guide
(define-param n-InP-1 3); indices of refraction
(define-param n-InP-2 2)
(define-param n-core 3.4)
(define-param n-AlGaAs 3.5)
(define-param InP-1 (* n-InP-1 n-InP-1)); dielectric constants
(define-param InP-2 (* n-InP-2 n-InP-2))
(define-param core (* n-core n-core))
(define-param AlGaAs (* n-AlGaAs n-AlGaAs))

(define-param InP-w 12); InP ridge width
(define-param InP-SH 7); InP substrate height
(define-param cladding 0.5); AlGaAs cladding height
(define-param core-h 2)
(define-param top-h-1 2); top InP layer heights
(define-param top-h-2 1)

(define-param InP-l (+ (* 0.5 (- sx d)))); dimensions of the waveguide
(define-param InP-x-center (+ (* -0.25 sx) (* -0.25 d )))

; all relating to the SOI rib waveguide
(define-param n-Si 3.47772); index of refraction
(define-param n-SiO2 1.5277)
(define-param Si (* n-Si n-Si) ); dielectric constant
(define-param SiO2 (* n-SiO2 n-SiO2) )

(define-param Si-h 3.7); silicon etch depth
(define-param Si-H 8.2); silicon top layer height
(define-param Si-SH 0); silicon substrate height
(define-param ox-h 6); height of the oxide layer
(define-param Si-w 8); width of the SOI waveguide

(define-param Si-l (+ (* 0.5 (- sx d)))); dimensions of the waveguide
(define-param Si-x-center (+ (* 0.25 sx) (* 0.25 d )))

(define-param horn-l 10)
(define-param horn-w 14)
(define-param horn-center-x (+ (* 0.5 d) (* horn-l 0.5))
(define-param horn-center-y (+ (* -0.5 sy) ox-h Si-H (* -0.5 Si-h) ) )

(set! geometry
  (list
   ; InP layers
   ; Substrate
   (make block (center InP-x-center (+ (* -0.5 sy) (* 0.5 InP-SH)) 0)
   (size InP-l InP-SH infinity)
   (material (make dielectric ( epsilon InP-1)))) )

; Cladding
;(make block (center InP-x-center (+ (* -0.5 sy) InP-SH (* 0.5 cladding)) 0)
;(size InP-l cladding InP-w )
;(material (make dielectric (epsilon AlGaAs)))

; Core
(make block (center InP-x-center (+ (* -0.5 sy) InP-SH cladding (* 0.5 core-h)) 0)
(size InP-l (+ core-h 1) InP-w )
(material (make dielectric (epsilon core))))

; Cladding
(make block (center InP-x-center (+ (* -0.5 sy) InP-SH cladding core-h (* 0.5 cladding)) 0)
(size InP-l cladding InP-w )
(material (make dielectric (epsilon AlGaAs))))

; Top layer 1
(make block (center InP-x-center (+ (* -0.5 sy) InP-SH (* 2 cladding) core-h (* 0.5 top-h-1)) 0)
(size InP-l top-h-1 InP-w )
(material (make dielectric (epsilon InP-1))))

; Top layer 2
(make block (center InP-x-center (+ (* -0.5 sy) InP-SH (* 2 cladding) core-h top-h-1 (* 0.5 top-h-2)) 0)
(size InP-l top-h-2 InP-w )
(material (make dielectric (epsilon InP-2))))

; SOI waveguide
; substrate (no thickness atm)
(make block (center Si-x-center (+ (* -0.5 sy) (* 0.5 Si-SH)) 0)
(size Si-l Si-SH infinity)
(material (make dielectric (epsilon Si))) )

; Oxide layer
(make block (center Si-x-center (+ (* -0.5 sy) Si-SH (* 0.5 ox-h)) 0)
(size Si-l ox-h infinity)
(material (make dielectric (epsilon SiO2))) )

; Si Top layer
(make block (center Si-x-center (+ (* -0.5 sy) Si-SH ox-h (* 0.5 Si-H)) 0)
(size Si-l Si-H infinity)
(material (make dielectric (epsilon Si))) )

; etch to make the ridge
(make block (center Si-x-center (+ (* -0.5 sy) Si-H ox-h Si-SH (* -0.5 Si-h))
(+ dz (* 0.5 Si-w) (* 0.25 (- sz Si-w))) )
(size Si-l Si-h (* 0.5 (- sz Si-w)))
(material air) )
(make block (center Si-x-center (+ (* -0.5 sy) Si-H ox-h Si-SH (* -0.5 Si-h))
    (+ dz (* -0.5 Si-w) (* -0.25 (- sz Si-w))))
(size Si-l Si-h (* 0.5 (- sz Si-w)))
(material air)
)

(make block (center horn-center-x horn-center-y dz) (size horn-l Si-h horn-w)
(material (make dielectric ( epsilon Si)))
)

(make block (center horn-center-x horn-center-y (+ dz 7)) (size 11 Si-h 2.87)
(e1 -10 0 3) (e2 0 1 0) (e3 3 0 10) (material air)
)
(make block (center horn-center-x horn-center-y (+ dz -7)) (size 11 Si-h 2.87)
(e1 -10 0 -3) (e2 0 1 0) (e3 -3 0 10) (material air)
))

(set! pml-layers (list (make pml (thickness t))))

(set! sources (list
    (make source
        (src (make gaussian-src (frequency f) (fwidth df)))
        (component Ey) (center (+ (* -0.5 sx) t) 0 0)
        (size 0 8 8 ))))

(set-param! resolution 10)

(define trans ; transmitted flux
    (add-flux f df nfreq
        (make flux-region
            (center (- (* 0.5 sx) t) 1.1 dz)
            (size 0 8.2 8))))

(run-sources+
    (stop-when-fields-decayed time Ey
        (vector3 (- (* 0.5 sx) t) -1.1 0 ) 1e-3)
    (at-beginning output-epsilon))

(display-fluxes trans)
APPENDIX C:

FABRICATION RECIPES

C.1 Copper Electroplating

In the electrolytic plating, mixture for bottom-up plating solution containing a relatively large, slow diffusing, suppressive additives (e.g. polyethylene glycol), is used. We also combine another additive (e.g. a kind of organic sulfur compound) that preferentially adsorbs within the trenches and speeds up the plating rate. We use electrolytic copper plating solvent InterVia Cu 8520 from Rohm and Haas. The solvent has excellent micro via hole filling performance, and supports pulse and reverse-pulse current plating. This InterVia Cu 8520 bath comprised of three solutions: InterVia Cu 8500, 8520A and 8520C. InterVia Cu 8500 is a basic solution that contains copper sulfate (CuSO₄·5H₂O) (providing copper ions); sulfuric acid (providing a plating solution with conductivity and leveling effect); and chloride (necessary to promote dissolution at the anode and affects the deposition reaction at the cathode). On the other hand, InterVia Cu 8520A and 8520C are organic additives, which improve plating properties and filling performance of the film. The make 1 liter of the bath we add 984 ml of InterVia Cu 8500, 1.5 ml of InterVia Cu 8520C, and 15 ml of InterVia Cu 8520A and then mix them well.
We used an industry standard phosphorized copper (0.055%) from IMC as the anode. For electroplating, we choose pulse-reverse current to improve high-aspect-ratio features. A alternating pulse current is used. The forward pulse current is 0.083 A/inch\(^2\), with on time of 2.5 ms and off time of 0.5 ms, and the reverse current is 0.023 A/inch\(^2\), with on time of 0.3 ms and off time of 0.7 ms. The current is chosen based on the plating bath and the power supply. The power supply used by us is a DuPR 10-1-3 from Dynatronix. With the current flow recipe mentioned above, it takes around 2 hours to fill up 15 μm deep nodule trenches. As the sample is covered with the Kapton tape, the waveguide portion of the sample does not accumulate any electroplated Cu on top of it.
C.2 AZ 4620 Recipe for Lithography

The photolithography recipe of the AZ 4620 resist is given below:

1. Spin Speed and Time - 2000 rpm for 40 seconds
2. Pre-exposure bake - 120\(^{\circ}\) C for 5 minutes (7 minutes after the second spin if double spin is done)
3. Exposure time: 90 seconds for single spin/ 180 seconds for double spin
4. Develop: 225 seconds for single spin/ 600 seconds for double spin in AZ 400K 1:4 (pre-diluted)
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